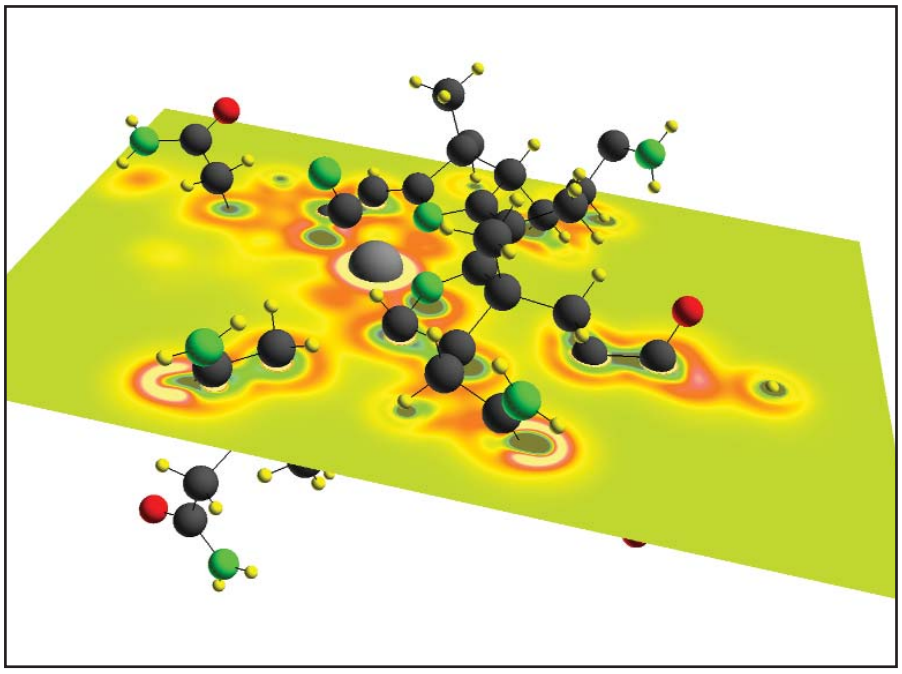
Fall 2001

Gridpoints

The Quarterly Publication of the NASA Advanced Supercomputing Division



NAS researchers are developing a software component for mesh and field data known as Field Model to enable the sharing of data from a variety of scientific disciplines. See page 9

FEATURES

Solving The Cancer Equation — 4

The Heat Is On . . . Earth — 6

Special Section: NASA at SC2001 — 1A

Field Model: Developing A Scientific Data Model — 9

Air Traffic Control Using Wake Vortex Management — 14

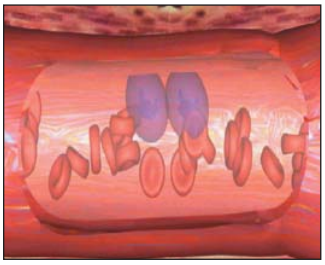
Features

4

Solving The Cancer Equation

A visiting professor at the NAS Division believes the key to winning the war against breast cancer is using partial differential equations to model the spread of cancer in individuals.

Holly A. Amundson

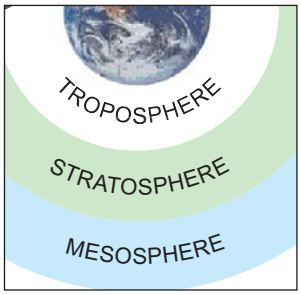


6

The Heat Is On. . . Earth

Computational Chemistry is being used to calculate the level of toxicity of industrial compounds being released into the Earth's atmosphere, which are contributing to a rise in global surface temperatures.

Holly A. Amundson



1A

NASA At SC2001: Demonstration Listing

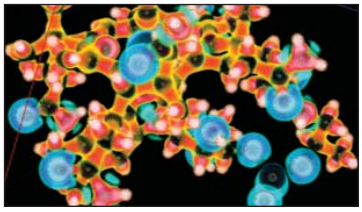
Researchers from six NASA centers gather in Denver to showcase their work in high-end computing, networking, and visualization. Special 12-page insert begins following Page 8.

9

Field Model: Developing A Data Model For Scientific Data

Field Model is designed to enable the sharing of data from a variety of scientific disciplines, as well as increase reuse of analysis and visualization software components.

Patrick J. Moran



14

Air Traffic Control Through Wake Vortex Management

Theories advanced by the NAS Division's Physics Simulation and Modeling Office will increase airport capacity by reducing aircraft spacing in bad weather.

Nicholas A. Veronico

On The Cover:

NAS researchers have developed the Field Model for data sharing and visualization across scientific disciplines. Volume rendering of a vitamin B-12 molecule. For more information, turn to page 9. (Chris Henze)

Gridpoints
The Quarterly Publication of the NASA Advanced Supercomputing Division

Vol. 2, No. 3 • Fall 2001

Executive Editors: Bill Feiereisen, John Ziebarth

Editor: Nicholas A. Veronico

Writers: Holly A. Amundson, Jill A. Dunbar, Patrick Moran

Graphic Designer: Sue Kim
Illustrator: Gail Felchle
Photographer: Michael Boswell

Contact the Editor:
Nicholas A. Veronico
Gridpoints
M/S 258-6
Moffett Field, CA 94035-1000
Tel. (650) 604-3046
Fax (650) 604-4377
nveronico@mail.arc.nasa.gov

The staff of *Gridpoints* would like to thank the following people for their assistance in preparing this publication: David Alfano, Dick Anderson, Bryan Biegel, Michael Boswell, Johnny Chang, Jill Dunbar, Chris Gong, T.R. Govindan, Chris Henze, Daniel Herr, Mary Hultquist, Bill Johnston, Randy Kaemmerer, Sue Kim, Chris Kleiber, Tim Lee, Marco Librero, Y.K. Liu, Nagi Mansour, Meyya Meyappan, George Myers, Terry Nelson, Marcia Redmond, Karim Shariff, Ryan Spaulding, Leigh Ann Tanner, Scott Thompson, Malu Trehan, Arsi Vaziri, Cliff Williams

Gridpoints is a quarterly publication of the NAS Advanced Supercomputing Division at NASA Ames Research Center. The division's staff includes government employees and contractors from Advanced Management Technology Inc., Computer Sciences Corp., Cray Inc., Eloret, Raytheon Co., and SGI.

Subscribe to *Gridpoints*

Subscriptions to *Gridpoints* are complimentary. Please send e-mail with your name, company name, title, address, and zip code to:
gridpoints@nas.nasa.gov
or subscribe online at:
www.nas.nasa.gov/gridpoints/subscribeform.html

Note: Subscribers outside the continental United States can access *Gridpoints* on the web in PDF format at: http://www.nas.nasa.gov/gridpoints

News From NAS

NAS Speeds New Rocket Turbine Design

Engineers at NASA's Marshall Space Flight Center (MSFC) were recently able to shave three-and-a-half months off the task of simulating a supersonic turbine, thanks to the work of NAS Division user services staff. The simulations were performed on supercomputers located at the NASA Advanced Supercomputing (NAS) Facility, to analyze the unsteady flow in an advanced turbine design. The results will help in the design of more efficient and durable rocket engines.

Responding quickly to a request from MSFC's Applied Fluid Dynamics Analysis Group, Chuck Niggley, NAS Scientific Consulting Group lead, and colleague Herbert Yeung, provided access to special computational resources when regular resources proved insufficient for the MSFC simulation task. The NAS team set up a special account for users, and worked around the clock to keep MSFC apprised of anticipated changes in the computing environment.

In a letter of thanks to NASA officials, Daniel J. Dorney, of MSFC's Applied Fluid Dynamics Analysis Group, said: "Both Chuck and Herbert should be complimented on their willingness to help users solve computer-related issues, their understanding of users deadlines, and their positive attitude."

Continued on page 2

NAS Mission

To lead the country in the research, development, and delivery of revolutionary, high-end computing services and technologies, such as applications and algorithms, tools, system software, and hardware to facilitate NASA mission success.

From The Division Chief

The NAS Division, in collaboration with our industry partner SGI, has installed and is now running a 1,024-processor single-system image (SSI) supercomputer. The SSI system is unique in that it uses a single operating system to control its 1,024-processors, a single shared memory, and the input/output subsystem. Division researchers had high expectations for how a number of scientific applications would scale on the new system. To date, we have run both aero- and Earth-science applications, and our scaling expectations have proven true. In addition, the 1,024-processor supercomputer uses the same operating system and compilers as our previous SSI machines, which enables scientists to transition to the new computer without losing valuable research time rewriting codes.

Bringing the 1,024 processor SSI supercomputer on line provides more powerful nodes enabling researchers to access remotely located computing resources, storage devices, and scientific instruments. NASA Administrator Dan Goldin has supported the division's strategy of developing a distributed computing environment, NASA's Information Power Grid (IPG) project, and enhancing the power of nodes on the grid.

A number of research projects made possible through the advancements in compute power are profiled in this issue. NAS Division computational chemists are collaborating with academic researchers to determine the global warming potentials of industrial compounds. This research will provide an insight into our planet's climate, and help determine what actions should be taken today to safeguard our future.

In the area of biomedicine, a visiting professor of mathematics from Eastern Illinois University is working with NAS researchers to develop mathematical models for predicting the spread of cancer cells in the human body, and how the cells can be contained. This research is focusing on breast cancer, a disease that attacks both men and women.

Members of the NAS Research Branch's Data Analysis Group, have developed the Field Model, a tool that allows researchers from different disciplines to share, visualize, and interact with computational data. In addition, the division's Physics Simulation and Modeling Office has patented a new method for reducing the spacing of aircraft on approach to landing. When adopted by industry, this spacing method will help increase airport capacity.

NASA will be showcasing a number of the division's research projects that have been brought to fruition through the use of high-end computers at the SC2001 conference in Denver, November 11-16. Our partners at five other NASA centers will join us to demonstrate the advancements achieved through computational science and high-speed networking. I invite you to stop by our booth to see this work firsthand, or view a brief synopsis of each research demonstration in the SC2001 insert following page 8.

As always, I welcome your feedback.

Bill Feiereisen
wfeiereisen@mail.arc.nasa.gov

Continued from page 1

MSFC has designed and experimentally tested a supersonic turbine, called the "Simplex" turbine. This "partial-admission" turbine (that is, the flow enters the turbine over only a portion of the turbine inlet) was designed as a ground demonstrator, and was experimentally tested with both metal and composite airfoils (blades) to study the feasibility and durability of advanced composite materials. "The experiments showed that the composite airfoils performed very well," said Dorney.

While the experiments yielded significant insight into the flow physics, an assessment of the unsteady flow field required the extensive use of three-dimensional simulations. The simulations were also intended to provide a better understanding of the flow physics of partial-admission turbines, often used in rocket engines. According to Dorney, the simulations were also used to validate NASA's CORSAIR code for partial admission and full-annulus simulations.

Although computational models normally consider only a portion of the 360-degree annulus of the turbine, the nature of the Simplex turbine required simulation of the full 360-degree annulus, modeling all of the airfoils, Dorney explained. The computational grid used in the simulations contained in excess of seven million grid points and required approximately two months of wall-clock time for each simulation.

Specific goals for these simulations were to determine the unsteady pressures experienced by the turbine airfoils to help interpret the experimental data and help determine the durability of the airfoils. Another goal was to determine the effects of a partial admission flow field on the performance of the turbine. The simulations served as precursors for many Space Launch Initiative tasks, which consider the use of partial admission turbines.

Division Engineers Address 802.11b Wireless Security Flaws In NAS Environment

The network group and information security group in the NAS Division have successfully installed a secure interoperable wireless network that addresses the well-known problems of the 802.11b standard wireless systems – with a minimum of time and investment.

"Wired equivalent privacy isn't the equivalent of wired privacy," said Dave Tweten, computer security official at NAS. The network group and information security group started with the premise that the network itself provides no reliable authentication and no security from eavesdropping, and decided not to depend on any security provisions bundled with 802.11b products.

Why? Recent conference results have established that 802.11b wireless systems provide no substantial security protection in any of three important respects: The signal coverage perimeter cannot be easily limited to conform to an organization's physical control perimeter; wireless card hardware addresses cannot be trusted as tools to identify a user; and Wired Equivalent Privacy (WEP) encryption of data sent between a laptop and an access point can be cracked, regardless of key length.

In addition, said Tweten, the means to derive a WEP encryption key from eavesdropped ciphertext and a method for decrypting WEP traffic without ever needing to derive the key are well documented.

The NAS Division chose to secure its wireless network while assuming that it would be accessible from areas outside the division's control. The team also assumed that all information on the network would be subject to eavesdropping, and that no identification information built into 802.11b could be trusted. "All 802.11b security features were disabled on the grounds that they only consume resources without delivering any real security," Tweten said.

For minimum administrative overhead, basic use of the wireless network is possible without authentication. This is possible because the services that can be reached require authentication and perform encryption themselves. At the same time, users are protected from an attack launched on the Internet at large.

In the NAS Division, this is accomplished by an off-the-shelf PC running the OpenBSD operating system, an Apache web server, the Internet Software Consortium Dynamic Host Configuration Protocol server, and the IPF (Internet Packet Filter) firewall software – all freeware. Network and security team members Nichole Boscia and Derek Shaw developed the "glue" software to make the rest of the components work together – in about 40 hours. For a copy of the Wireless Firewall Gateway White Paper, visit: www.nas.nasa.gov/ Research/ Tasks/Networks/Wireless/ whitepaper.html

Chimera Grid Tools Version 1.6 Released

A new version of the Chimera Grid Tools (CGT), a set of programs and scripts for generating overset grids, was released. Developed at Ames Research Center, CGT is widely used for solving complex computational fluid dynamics (CFD) problems in a variety of real-world applications, including aerospace, marine, automotive, environmental, and sports.

Among the many new capabilities for CGT version 1.6 are: read and animate body dynamics by reading from a dynamics table file, or from an arbitrary user routine; read CART3D triangles and q file (.triq) containing grid and scalar functions; display scalar functions on triangles in DIAGNOS; capability to run OVERFLOW-D to create off-

IPG Team Receives Prestigious NASA Award

NASA's Information Power Grid (IPG) team recently received the NASA Group Achievement Award, presented to selected groups who make outstanding contributions to the agency's mission. The NASA Advanced Supercomputing (NAS) Division is leading the effort to build and test the IPG, a network of high-performance computers, data storage devices, and scientific instruments. Ames is collaborating with colleagues at Glenn and Langley Research Centers on the project.

Ames Research Center Deputy Director William E. Berry, left, and Center Director Henry McDonald, far right, present the NASA Group Achievement Award to the Information Power Grid team, represented by Leigh Ann Tanner, IPG program manager, and Arsi Viziri, IPG deputy project manager. *(NASA/Dominic Hart)*

Presented at the annual NASA Honor Awards Ceremony on July 26 at Ames, the award cites the "successful implementation of Information Power Grid and completion of the first two level-one milestones" and recognizes that the IPG will become the service delivery model for high-performance computing for NASA. In fiscal year 2000, the IPG team demonstrated a complete version of a grid system and successfully performed high-speed data access on the grid's infrastructure. "I'm particularly happy with the (NAS) organization's tremendous progress over the three years that IPG has been underway," says NAS Division Chief William J. Feiereisen. "Our work is now being recognized in the world outside of NASA – people are looking to us to find out what to do in high-performance distributed computing."

"The IPG is becoming the model by which NASA accesses its high-performance computing resources," says IPG Project Manager William E. Johnston. "Three years ago we felt we had an opportunity to fundamentally change the way computing is done – and we have accomplished that." In late July, Johnston met in London with center directors for IBM's recently announced grid initiative to present grid implementation methods developed for the IPG.

The IPG has been a major project under NASA's Information Technology and High Performance Computing and Communications programs. For more information on NASA's Information Power Grid, visit www.ipg.nasa.gov.

body Cartesian grids; and perform domain connectivity compatibility with Tcl/Tk version 8.3.3. To get more details, and find out how to get CGT, contact co-developer Stuart Rogers in the NAS Division at rogers@nas.nasa.gov.

New Boron-Nitrogen Nanotube Research Published

A new development in the field of nanotechnology by NAS researcher Deepak Srivastava is described in *Physical Review B,* (Vol. 63, pg. 195413, 2001). In "Anisotropic Nanomechanics of Boron-Nitride Nanotubes: Nanostructured Skin Effect," Srivastava and colleagues Madhu Menon (University of Kentucky) and Kyeong Jae Cho (Stanford University) studied the way in which boron-nitride (BN) nanotubes respond to compressive strains, and their mode of plastic deformation. Their findings show that BN nanotubes may be useful as reinforcing fibers in ultra-light and strong functional composite materials. Additionally, such a material will exhibit an anisotropy against external axial strains – when the nanotube structure is compressed from both sides, damage occurs to one side only. "We have discovered an "anisotropic" mode of axial load transfer in strained BN nanotubes," says Srivastava. Based on this finding, the team has proposed a "skin-effect" model of nanocomposite materials with parallel-aligned zig-zag BN nanotubes. "Such material, if fabricated, would limit structural damage to the "skin" side of the material and not the inner core side," Srivastava explains. "One application, for example, might be to someday use this material in auto manufacturing, where damage in a collision could potentially be limited to the outside of the vehicle."

Srivastava and collaborators are now investigating the characteristics of nanotube-reinforced polymeric materials. BN nanotubes could be tested as reinforcing fiber simulations in functionally smart polymer composite materials of the future. If such a hypothetical material were fabricated, it would have numerous useful applications in transportation, aerospace, and defense.

Solving The Cancer Equation

A visiting professor at the NAS Division believes the key to winning the war against breast cancer is using partial differential equations to model the spread of cancer in individuals.

Breast cancer currently plagues more than two million women in the United States – a startling 12.5 percent of women in California alone. Suhrit K. Dey, professor of mathematics at Eastern Illinois University, is currently collaborating with computer scientists in the NASA Advanced Supercomputing (NAS) Division to create mathematical models that will predict how cancer spreads in the human body, and how it may be contained or even cured.

Dey plans to integrate a technique called multi-level parallelism (MLP) into his three-dimensional modeling code to enhance its computational performance on the NAS Division's 512-processor SGI Origin 3800 supercomputer, *Lomax*. Dey's mathematical models are based, in part, on his theory that there is a direct correlation between stress levels and the development of breast cancer (see Figure 1).

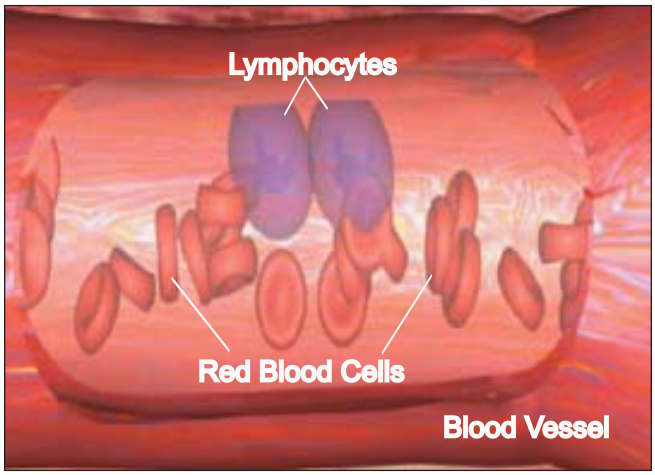


Figure 1: *Lymphocytes play a very important role in our immune system by seeking out and destroying cancer cells. When a person is under stress, hormones like glucocorticoid are released into the blood stream, which significantly reduces the number of lymphocytes present to fight off cancer cells. The figure shows extremely slow cloning, or reproduction of lymphocytes in the bloodstream as a result of stress.*
(Visualization by Cliff Williams/NASA)

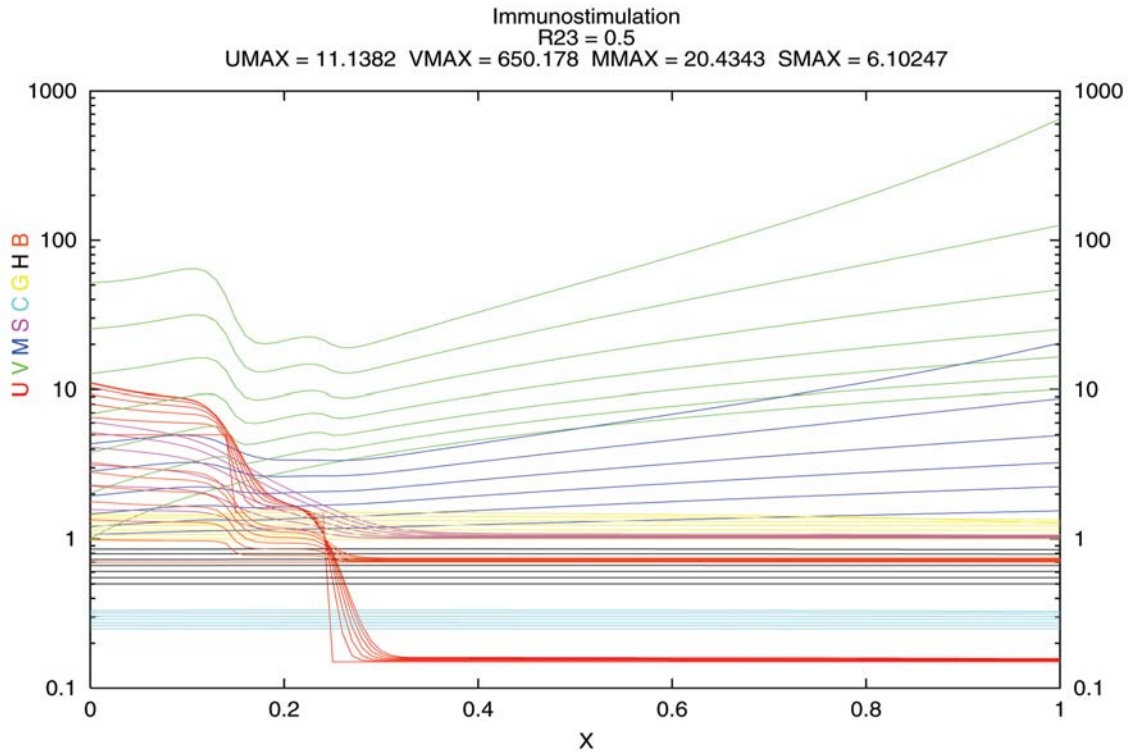
Dey is currently computing one-dimensional cancer models using a set of eight mathematical equations. These models include several variables such as the number of lymphocytes (cells in the human body that attack cancer), number of cancer cells, types of medical treatments, angiogenesis (the development of new blood vessels), and glucose levels in the body (see Figure 2, page 5). "I am building these models based on information I'm gathering in scientific journals, which is qualitatively accurate. Once the models are complete, I will input an individual's data to provide us with some quantitative results – this will enable us to predict if that individual will get cancer, or if their body's immune system can revert the process," explains Dey.

"Right now the problem I am solving is on a small scale, but I am getting some qualitatively valued results which help me communicate better with medical doctors," says Dey. After presenting his theory about the correlation between stress and breast cancer, Dey has received a tremendous amount of support from the medical community.

"I feel that Dr. Dey's approach is both novel and intriguing, and could lead to important developments in this field. What he offers is an overview approach that will give mathematical weight to many specific factors involved in causing, preventing, and treating cancer," says Dr. Steven Oppenheimer, director of the California State University at Northridge's Center for Cancer and Developmental Biology.

The Three-Dimensional Approach

Dey is currently seeking a grant that will allow him to begin generating three-dimensional cancer growth models. These models will solve more than 16 million mathematical equations used to describe cancer growth. NAS computer scientists Jim Taft and Rupak Biswas are slated to parallelize Dey's cancer modeling code to run on *Lomax*, and will also assist him with the integration of the multi-level parallelism technique, developed by Taft. Using three-dimensional cancer models enabled by MLP, Dey will be able to predict the rate of breast cancer growth and/or decay in an individual based



(U) Red = number of cancer cells • (V) Green = number of lymphocytes, or T-cells • (M) Dark blue = medication used to assist thymus function • (S) Purple = medication that kills both cancer cells and lymphocytes • (C) Aqua = carcinogens • (G) Yellow = glucose • (H) Black = medication that limits the amount of glucose consumed by cancer cells • (B) Orange = vascularization (excessive growth of blood vessels that provide the cancer cells with more nutrients to grow)

Figure 2: *Immunostimulation (the activation of lymphocyte production) may be achieved through relaxation techniques (such as yoga and meditation), regular exercise, diet, and/or some medications. When the immune system is strong, the body is able to stop the growth of cancerous tumors. Reading the graph from right to left, the number of lymphocytes (green) is greater than the number of cancer cells (red) — in this case, the immune system is able to conquer cancer. (Suhrit Dey)*

on their condition – levels of stress, amount of exercise, and food intake, for example.

In order to create a fairly accurate cancer prediction model, all factors or conditions involved, such as the size of the tumor and level of carcinogens in the body, must be considered at the same time. Since MLP is a shared memory technique, meaning all blocks of work have access to the same area of memory on the computer simultaneously, it is ideal for the cancer modeling code. "The kinds of problems that Dey is doing require very rapid communication between different parts of the calculation in parallel – MLP will be able to do this very efficiently. The fundamental construction of Dey's code structure is very similar to that of NASA's computational fluid dynamics code OVERFLOW-MLP, which contains many small blocks of work that have to communicate rapidly with each other. Because of these fundamental similarities, we expect the code to scale well with MLP," explains Taft.

Collaborative Efforts Are A Must

Although Dey is returning to Eastern Illinois University at the beginning of August, after a five-month visit at Ames, he will continue collaborating with Taft and Biswas to carry out his 3-D modeling work on *Lomax*. Once these models are complete, Dey is planning to collaborate with mathematics professor Glenn Webb at Vanderbilt University to expand on the cancer prediction models. "Dr. Dey is developing elaborate models of tumor growth, incorporating multiple features of tumor cell and immune cell interactions. The most interesting feature of these models is their exploration of the importance of the immune system in controlling tumor growth," says Webb, who has been working on mathematical modeling of cancer for 30 years.

Although Dey's mathematical models for cancer prediction are qualitatively accurate, they are designed only to accompany clinical studies on breast cancer, not to replace them. "We need a combination of mathematical models, statistical models, and clinical studies, so we can see breast cancer from every possible angle. I can see the light at the end of the tunnel. The solution is there, but desperately, I need help from others so breast cancer can be contained," says Dey. "If 10 percent of the people take an interest in this and protect themselves, that's a large number of women being saved."

—Holly A. Amundson

Editor's note: *Suhrit Dey welcomes and appreciates questions and/or suggestions. Contact him at: cfskd@ux1.cts.eiu.edu, or visit his website: www.ux1.eiu.edu/~cfskd*

The Heat is on...Earth

Computational Chemistry is being used to calculate the global warming potential of industrial compounds being released into the Earth's atmosphere, which are contributing to a rise in global surface temperatures.

The Earth may become one hot potato if pollution-induced global warming continues to progress at its current rate. Scientists at the U.S. National Center for Atmospheric Research in Boulder, Colorado, predict global temperatures will rise one to two degrees Fahrenheit within the next 30 years, and three to nine degrees during this century. Such temperature increases will have devastating effects on the planet, causing polar ice caps to melt and raising sea levels, which will lead to flooding. Timothy Lee, from the computational chemistry group in the NASA Advanced Supercomputing (NAS) Division, is collaborating with Professor Joseph Francisco from Purdue University, West Lafayette, Indiana, to study compounds released in the atmosphere by industry and how they are contributing to the amplified effects of global warming.

According to Lee, if there was no greenhouse effect, the surface temperature of the Earth would be approximately zero degrees Fahrenheit, and the environment would be unable to sustain human, animal, and plant life as we know it. Through the greenhouse effect, (see Figure 1, page 7) the Earth's surface temperature is raised to about 58 degrees Fahrenheit on average. The Earth radiates part of the energy sent from the sun back into space though the atmospheric window, which is defined as a set of wavelengths on the electromagnetic spectrum between 700 and 1,500 wave numbers (cm^{-1}). In 1970, the radiation emitted from Earth was measured during NASA's *Nimbus 4* Infrared Spectroscopy Experiment. The problem arises when gases in the atmosphere, such as carbon dioxide, absorb too much radiation in the window region, preventing it from escaping into space. Heat trapped by greenhouse gases travels back to the Earth's surface, resulting in a significant rise in global temperature. "Current research is showing that there is a strong link between an increase in surface temperature and greenhouse gases," says Francisco.

"The atmosphere is trapping energy that the Earth is transmitting, and reflecting some of the energy back to the surface because it can't escape through the atmospheric window," explains Lee. "We need the Earth to release some of this energy, otherwise the surface temperature will rise higher than it is now."

Finding the Potential

To determine whether a particular compound in our atmosphere is contributing to the increase in global temperatures, Lee and Francisco calculate the global warming potential (GWP) of compounds using computational quantum chemistry methods – an approach to chemistry using mathematics and computers to describe chemical reactions and the radiation properties of molecules. The GWP of a compound is a measure of its impact on global warming over time as a result of the release of a given amount of the greenhouse gas into the atmosphere.

Compounds with large GWPs have a significant impact on global warming, and generally have three characteristics: the compound absorbs infrared radiation in the atmospheric window region (instead of allowing the radiation to pass through the window into space); absorption coefficients in the window region are very high; and the compound has a long atmospheric lifetime. All molecules possess characteristic vibrational frequencies, which may absorb infrared radiation depending on their absorption coefficients or infrared intensities. The characteristic vibrational frequencies of a given compound can be determined through quantum chemistry calculations. Using such calculations, Lee and Francisco have been able to explain why compounds like perfluorocarbons meet all three of GWP criteria, and therefore have significant global warming potentials.

Compounds containing fluorine, for example, are always going to have vibrational frequencies that lie in the atmospheric window because their stretching frequencies (dependent upon the bond strength and masses of the atoms) are within the atmospheric window region. "A typical carbon-fluorine stretch, for example, is around 800 cm^{-1} – which falls within the atmospheric window," explains Lee.

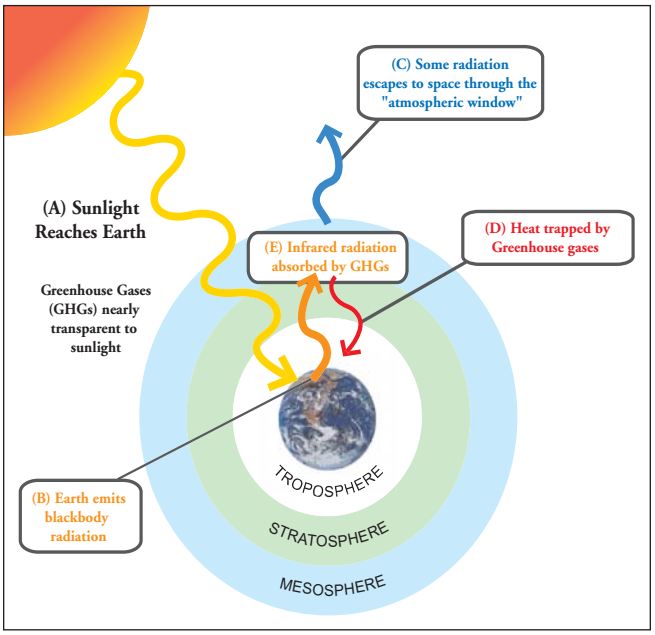


Figure 1: *Ultraviolet radiation travels from the Sun to the Earth's surface, and some of this radiation is absorbed by the surface, heating the planet (A). The Earth then emits blackbody radiation in the infrared spectral region (B). Some of the emitted radiation escapes through the "atmospheric window" into space (C). However, the remaining radiation is prevented from escaping by greenhouse gases (GHGs) such as carbon dioxide, water, ozone, and other trace compounds, which causes additional heating (D). The greenhouse effect is a natural process; however, the greenhouse effect has been increased by the release of dangerous compounds into the atmosphere from industrial sources, which absorb strongly in the "atmospheric window" (E).*

Having an absorption in the window region, however, is not enough to produce a significant global warming potential – the compound must also meet the second point of the GWP criteria that requires it to have a considerable absorption coefficient, or infrared radiation intensity, to have an impact. Fluorine, by nature, is a very electro-negative element – when it is bonded to a weakly electro-negative or electro-positive atom (as is the case with perfluorocarbons), it creates a highly polar bond, or a large "movement" of charge from one atom to another during the course of a stretching vibration. Generally, the more polar the bond, the more radiation is absorbed by the stretching vibration.

The third important component contributing to a large global warming potential is the atmospheric lifetime. Compounds that linger in the atmosphere for more than one year, and in some cases in excess of 100 years, have a large global warming potential, provided the other conditions are met. Generally, atmospheric lifetimes of compounds are based on reaction rates with hydroxyl radicals; the main scrubbing agent the atmosphere uses to break compounds down through chemical reactions. "Studies have shown that reactions between hydroxyl radicals and perfluorocarbons are very slow – they don't react very well at all," explains Lee. "And when hydroxyl radicals react slowly with a compound to break it up, it remains in the atmosphere for a long time."

Compounds composed of more hydrogen atoms tend to react faster with hydroxyl radicals (with methane being an exception) relative to compounds such as perfluorocarbons, which do not contain hydrogen atoms (perfluorocarbons are composed only of carbon and fluorine atoms). Perfluorocarbons generally have an atmospheric lifetime of tens of years, and in some cases, hundreds of years. "To solve the problem, we must figure out what we can and can't release

Global Warming vs. Ozone Depletion

"Compared to ozone depletion, the level of understanding of global warming is completely different — with ozone depletion, there's no question that humankind's activities are having a direct impact. With global warming, there are only certain things you can deduce — if you release compounds with significant global warming potentials in the atmosphere that are going to hang around for a 1,000 years, even in small amounts, it's going to build up and cause problems," explains NAS researcher Timothy Lee.

The physical processes of global warming and ozone depletion are very different. Global warming involves the release of compounds into the atmosphere that absorb radiation and trap it in the form of heat. Ozone depletion involves chemical reactions that destroy ozone molecules in the stratosphere, exposing Earth to high levels of the Sun's high-energy radiation. The ozone molecule is important to life on Earth, because it absorbs the majority of high-energy radiation from the Sun, preventing it from hitting the Earth's surface.

Ozone depletion occurs in the stratosphere – where the ozone, which protects Earth from the Sun, is located. Global warming occurs throughout the atmosphere, although Lee and Francisco's research is mainly concerned with the troposphere (see Figure 1, above). According to Lee, most of the compounds that cause ozone depletion also have global warming potentials. These compounds are non-toxic to humans, but quite detrimental to the ozone layer. Ironically, some of the compounds that industry is now using that were created to serve as chlorofluorocarbon alternatives (such as aerosol propellants in hair spray cans) to reduce ozone depletion will have a detrimental impact on global warming.

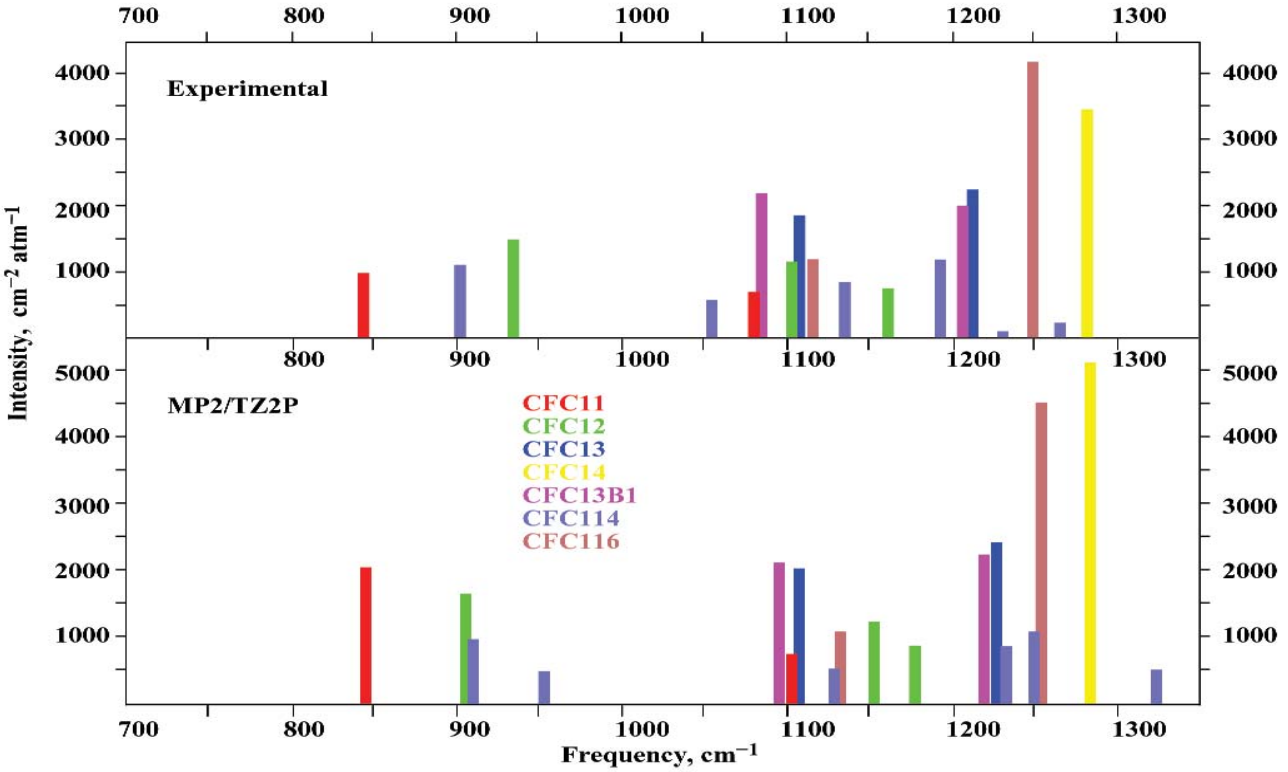


Figure 2: *Comparison of experimental results to computational chemistry calculations for the determination of chlorofluorocarbon (CFC) infrared radiation absorptions in the atmospheric window region, 700 to 1,500 cm^{-1}. Experimental data for CFCs were used to benchmark the computational chemistry approach for calculating infrared intensities.*

from the Earth's surface and then let the planet take care of maintaining the atmosphere's balance," adds Lee.

A Unique Approach

Lee and Francisco's use of computational quantum chemistry, rather than "traditional laboratory chemistry" is a new approach to calculating global warming potentials. "We conduct experiments on the computer – our laboratory is the computer," explains Lee. "Some experiments are not easily done in traditional labs, for example, in ozone depletion chemistry, compounds that are stable in the stratosphere are not stable at the Earth's surface; the computer enables us to carry out these otherwise dangerous experiments. For global warming studies, infrared intensities are difficult to measure in the lab, but are very straightforward to determine accurately using computational quantum chemistry methods." Lee and Francisco are calculating global warming potentials for fluorinated and chlorinated compounds such as chlorofluorocarbons (CFCs), hydrofluorocarbons (HFCs), hydrochlorofluorocarbons (HCFCs), and perfluorocarbons (PFCs), as well as others (see Figure 2).

"If you let certain compounds into the atmosphere, they have the potential to slam the atmospheric window shut – that would have a devastating impact," explains Lee. "The current challenge for scientists is designing new materials that meet the constraints of having low ozone depletion potentials, low global warming potentials, low toxicity, and yet are still effective for a particular industrial use," adds Francisco. The ultimate goal of Lee and Francisco's research is to help industry decrease or eliminate the release of dangerous compounds by using global warming potential data to guide new materials selection decisions.

"Understanding how bond types and number of bonds influence a molecule's global warming potential are essential to developing molecular design strategies to minimize the global warming ability of new materials," explains Francisco. "More importantly, it should give industry more flexibility and more options in developing environmentally benign materials."

Once Lee and Francisco complete their calculations of global warming potentials, they will publish their results in scientific journals, and pass them on to modeling experts. Scientific modelers will be able to incorporate Lee and Francisco's data into climate models demonstrating the effects of different compounds on global warming. Because very little research has been undertaken to determine the effects of perfluorocarbons and other fluorinated compounds on global warming, the impact that these compounds will have on global warming is not well appreciated nor well understood.

— Holly A. Amundson

Editor's note: *Srinivasan Parthiban, a former post doctoral student, also contributed to this research.*


SPECIAL EDITION
NASA at SuperComputing 2001
SC2001
SC2001
NASA
National Aeronautics and Space Administration
A look at NASA exhibits, events, and speakers at SC2001

Welcome, participants of SC2001.


Bill Ingalls/NASA

Daniel S. Goldin
NASA Administrator

As NASA Administrator, I am especially proud to welcome you to this important conference. The technical papers to be presented, the demonstrations to be seen and the professional friendships to be rekindled are exciting indeed. Gatherings such as this give us the opportunity to be refreshed and rejuvenated about our work. I am especially pleased to see that this conference not only features technical demonstrations, exhibits, and presentations, but that it also includes educational outreach. Thank you to the corporate and academic partners who are making this aspect of the conference possible.

Education is more important than ever. I have grave concerns about the future of America's leadership in science and technology because we have fewer and fewer young people entering technical fields. It is up to all of us, including the participants of this conference, to work with the high school and middle school teachers who are here to get young people interested–and excited–about technical fields, be it computing, networking, engineering, or...rocket science.

It is fitting that this year's conference, titled "Beyond Boundaries," is being held in Denver. This is a city poised at the base of the Rocky Mountains–that set of spectacular mountains over which our forefathers had to cross and endure as they continued the westward journey across this continent. We in technical fields in this country–mathematicians, scientists, engineers–face a formidable mountain range of sorts as we move through this new century...this new millennium. Without the influx of young people, of new blood and new ideas, our country is doomed to lose its leadership position in science and technology. So, give a special welcome to the teachers in your midst. Get to know them, work with them as we move through the Rocky Mountains of our millennium toward a promised land of opportunity for all.

Daniel S. Goldin

NASA is showcasing many of its exciting scientific research projects at SC2001. The following are descriptions of demonstrations, paper presentations, videos, and panel discussions listed by participating NASA researchers and collaborators.

Ames Research Center

Mountain View, California

As NASA's Center of Excellence for Information Technology, Ames Research Center (ARC) provides agency research leadership and world-class capability encompassing the fields of supercomputing and networking, high-assurance software development, verification, and validation, automated reasoning, planning and scheduling, and human factors.

NAS Grid Benchmarks

The NAS Grid Benchmarks (NGB) test the functionality and efficiency of Grid environments such as NASA's Information Power Grid. NGB extends the methodology of the NAS Parallel Benchmarks (NPB) to computational Grids. It consists of four distributed applications, the elements of which are NPB codes that exchange substantial data volumes.

The demonstration presents the first paper-and-pencil specification of the NGB, which can be used by Grid developers and operators to test their environment. These benchmarks also show prototype implementations using Java and the Globus Metacomputing Toolkit. NGB nominally measures turnaround time. The Globus implementation also reports queue time and CPU time.

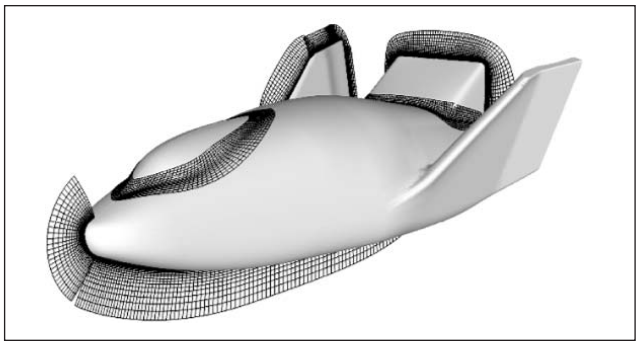
OVERSET Computational Fluid Dynamics Tools

This is a live demonstration of the NASA Ames OVERSET CFD software, including the Chimera Grid Tools, Overgrid, and Pegasus. Researchers will demonstrate complete grid-generation for a number of different applications from initial geometry definition to final preparation of all the inputs for the flow solution. For more information: visit: www.nas.nasa.gov/~rogers/home.html#software

ILab - Parameter Study Tool and Information Power Grid (IPG) Portal

The ILab tool was specifically written to solve the complex problems of creating and launching parameter studies. Though today's distributed computational resources are quite capable of running large parameter studies for aerospace problems, users have not had tools available that make this process easy and fast.

Within the last year, the ILab tool was given an intuitive user interface. Users can now specify their processes via an advanced CAD approach by visually constructing a flowchart-like graphic. ILab's code generator subsequently trans-

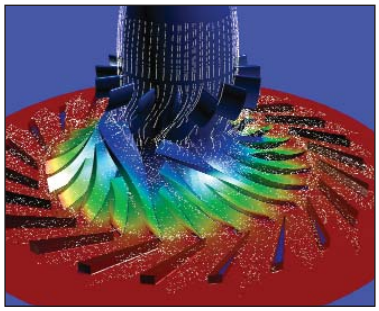


The NASA X38 Crew Return Vehicle was the subject of a two-dimensional parameter study in Mach number and angle-of-attack. ILab generated and submitted 192 separate flow field computations for the requested 16 values of Mach number and 12 values of angle-of-attack.
(NASA/Maurice Yarrow)

lates this into appropriate shell scripts, which are then launched onto remote systems and monitored. Researchers whose parameter studies consist of individual jobs with long-running computational fluid dynamics problems can now take advantage of ILab's unique "restart" capability. This allows users to automatically segment their jobs onto supercomputer scheduling systems and modify solver parameters for the purpose of steering the computation to a stable solution. Load balancing of jobs is automatically accomplished by restarting the jobs onto supercomputer systems with immediate processing availability. In addition, ILab has an advanced help system built-in, which users can access from any ILab screen.

Unsteady Turbopump For Reusable Launch Vehicle (RLV)

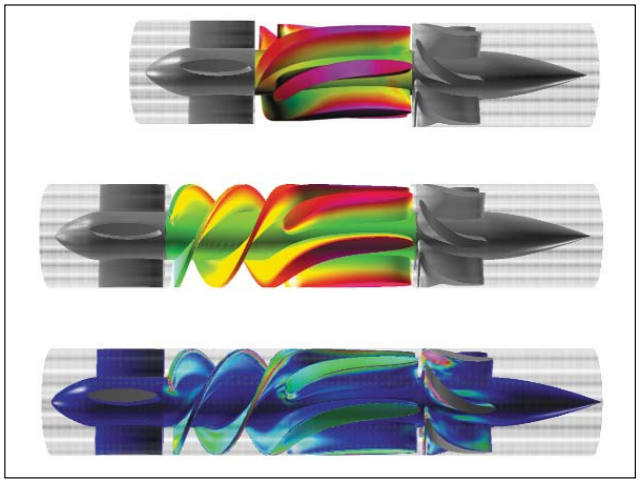
The objective of this effort is to provide a computational framework for design and analysis of the entire fuel supply system of a liquid rocket engine, including high-fidelity unsteady turbopump flow analysis. This is needed to support the design of pump subsystems for advanced space transportation vehicles that are likely to involve liquid propulsion systems. To date, computational tools for design/analysis of turbopump flows are based on relatively lower fidelity methods. An unsteady, three-dimensional viscous flow analysis tool involving stationary and rotational components for the entire turbopump assembly has not been available for real-world engineering applications. The present effort will provide developers with information such as transient flow phenomena at start up, impact of non-uniform inflows, and system vibration and impact on the structure.



Visualization of the entire fuel supply system of a liquid rocket engine, including high-fidelity unsteady turbopump flow analysis. (NASA)

DeBakey Heart Assist Device

Approximately 20 million people worldwide suffer annually from heart failure, a quarter of them in America alone. In the United States, an alarmingly low 2,500 donor hearts are available each year. The use of Computational Fluid Dynamics (CFD) technology has lead to major design improvements on the heart assist device, enabling its human implantation. NASA Ames scientists employed NASA Shuttle main engine technology and NASA CFD modeling capabilities, coupled with the NASA Advanced Supercomputing (NAS) Division's high-performance computing technology, to make several design modifications that vastly improved the heart device's performance.



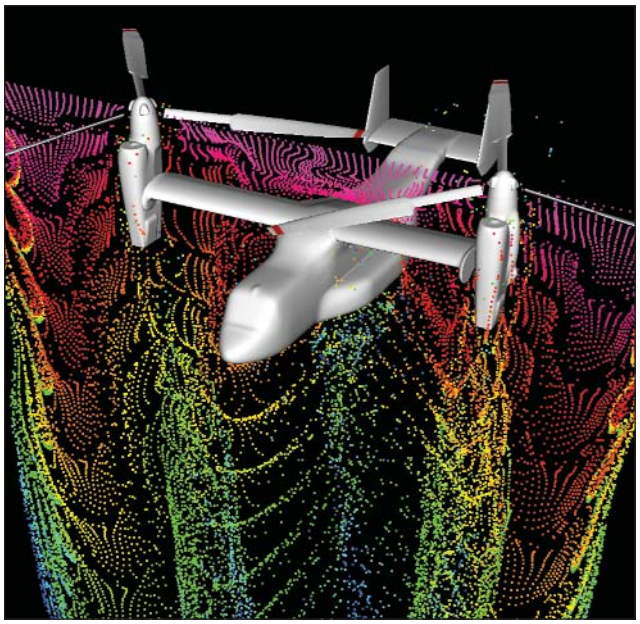
Visual comparison of the original ventricular assist device, top, and the unit after modifications by NAS researchers, lower. Adding an inducer to the DeBakey device eliminates the dangerous back flow of blood by increasing pressure and making flow more continuous. The device is subjected to the highest pressure around the blade tips, shown in magenta.
(NASA/Cetin Kiris)

Exploratory Computing Environments Component Framework

Exploratory computing environments is a component framework designed to enhance the ability of NASA scientists to visualize, analyze and interact with huge datasets and associated distributed computations. The components include a data model (Field Model (FM)), a metadata model (Active Metadata (AM)), a visualization technique library (VisTech), web technologies (Mars landing site problem solving environment), and distributed object technology (growler). Together, the components enable rapid prototyping and development of distributed computational environments. Application domains include aeronautics, earth science, biology and nanotechnology.

Parallel Distributed CFD for Unsteady Flows with Moving Overset Grids

The goal of this work is to develop techniques for parallel and distributed computations of large-scale unsteady moving body applications using overset structured grids. The flow domain is decomposed into a union of multiblock meshes, which may be in relative motion to one another.



Particle traces around a moving body problem. (NASA/M. Jahed Djomehri)

An approach based on the message-passing Chimera paradigm has been implemented in the OVERFLOW-D code with the Globus-MPICH-G toolkit that extends the execution environment to the IPG. Performance assessment of a large-scale Navier-Stokes problem consisting of a moving body grid system (approximately 37 million points) indicates the feasibility of wide area networks for this class of applications.

Mars Surveyor Landing Sites "Collaboratory"

Marsoweb is as a web-based interactive archive of data for selection of landing sites for the 2003 Mars Explorer Rover missions. This archive allows visual navigation of the candidate landing sites and various maps of data from the current Mars Global Surveyor (MGS) mission and from the Viking missions, including high-resolution images of the candidate sites. VRML scenes allow the user to roam the data in 3-D on the web. Marsoweb also features interactive archives of global data, which enable users to query MGS

Marsoweb home page at: http://marsoweb.nas.nasa.gov/landingsites.

IP Multicast for Seamless Support of Remote Science

Scientific investigations at remote locations on Earth can be tremendously enhanced by connectivity to existing networks that use standard protocols. This demonstration showcases the capability to both send and receive high-fidelity images using Internet Protocol (IP) multicast (via geosynchronous satellites) with the NASA Research and Education Network/Glenn Research Center (NREN/GRC) Transportable Earth Station (TES). A 20 Mbps IP multicast of previously stored video content is sent via satellite from a server at GRC to client machines at SC2001. With IP multicast, the satellite and network capacities are used optimally, regardless of the number of participants, yet the distribution of the signal can be limited to a specific group. For more information, visit: http://www.nren.nasa.gov

Ready access to high quality imagery and data improves the performance of remote scientists and increases the quality of their results. (NASA)

data maps and geology maps. Current development efforts include remote collaboration features and Venus topography data. For more information, visit: http://marsoweb.nas.nasa.gov/landingsites

Debugging on the Information Power Grid

This demonstration showcases three aspects of debugging on the Information Power Grid. First, researchers will show how a debugger can control the execution of a computation running on a heterogeneous collection of machines. This is a key requirement of a debugger for computational grids. Second, researchers will demonstrate how the debugging of tool-parallelized codes can be mechanized through the use of dependence analysis information, and a relative debugging approach that compares the executions of the parallel and serial codes. Finally, trace information collected during a computation will be used to provide a number of highly useful debugging operations. For more information, visit: www.nas.nasa.gov/Tools/p2d2/SC01

Control and Observation in Distributed Environments

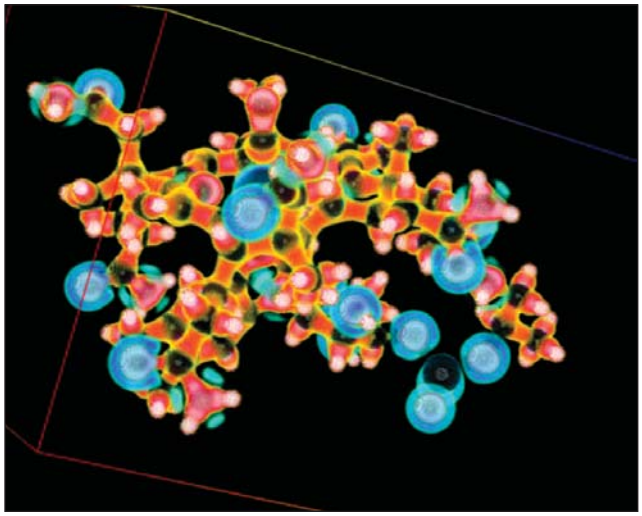
Researchers in the NAS Division at NASA Ames Research Center have developed a software framework, called CODE, for control and observation in distributed environments. This program allows researchers to observe and control resources, services, and applications in large-scale distributed systems. CODE provides a secure, scalable, and extensible framework to make observations, reason about observations, and perform actions to adjust how an observed entity is operating.

Administrators can use CODE to manage a computational grid by observing the resources and services that make up a grid and controlling their operation. In ongoing work, NAS researchers are using the CODE framework to provide grid information to a searchable, distributed directory service available to grid users. For more information, visit: www.nas.nasa. gov/~wwsmith/CODE

'growler' Visualization Tool

The "growler" environment provides an infrastructure that allows various kinds of functional modules to be "wired" together to create distributed and collaborative scientific applications. The individual components can be local or remote – that is, an application can be installed on a single machine, or it can be distributed over a network. Scientific visualization applications are typically decomposed into viewer components and data components. The viewers perform graphics and take in user input. The data components provide data – either from archival databases, from ongoing simulations, from instruments, from analysis procedures, or from some combination of these.

The growler environment allows researchers to combine a diversity of viewer and data components in order to create



Visualization of a vitamin B-12 molecule using the growler application. (NASA/Chris Henze)

a wide variety of custom-tailored utilities. For example, multiple viewers can be attached to a data stream to create a collaborative facility. Or a single viewer can receive input from multiple data sources, creating a single "console" for overseeing control and results from a multi-stage, distributed computation.

John H. Glenn Research Center

Cleveland, Ohio

Glenn Research Center (GRC) is NASA's Lead Center for Aeropropulsion and Center of Excellence in Turbo-machinery. GRC is committed to developing innovative technology and leveraging its computational, analytical, and experimental expertise in turbomachinery to future aerospace programs. GRC's aeropropulsion program plays a significant role in promoting safe and environmentally compatible U.S. aircraft propulsion systems.

NPSS: NASA Software of the Year

The Numerical Propulsion System Simulation (NPSS) Version 1 was selected co-winner of the NASA Software of the Year Award for 2001. Numerical Propulsion System Simulation Version 1 also received the NASA Office of Aerospace Technology Turning Goals into Reality Award for Goal 3 Pioneering Technology Innovation.

NPSS Version 1 is a world-class propulsion system simulation tool that provides the user with unprecedented capability and ease of use. NPSS Version 1 is an emerging U.S. standard for aerospace simulations. NPSS Version 1 is the first major aerospace design and analysis tool developed and written in the object-oriented (OO) programming paradigm to improve engineering productivity. NPSS' new OO software architecture enables multi-fidelity analysis in the design environment and facilitates integration of multiple disciplines. For more information, visit: http://hpcc.lerc.nasa.gov/npssintro.shtml

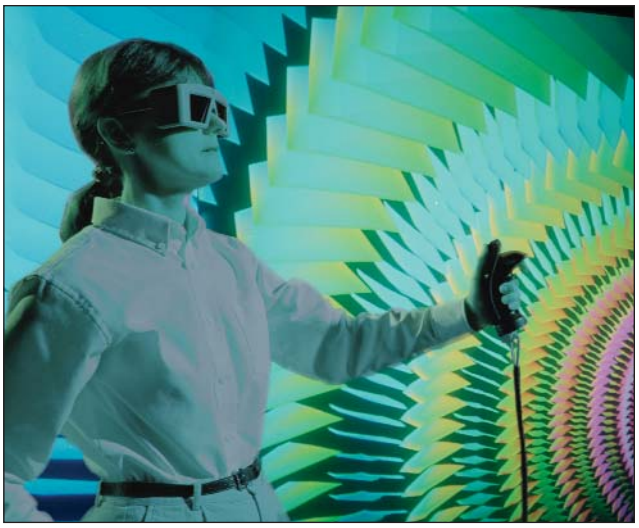
Project Integration Architecture: CAD Geometry Capture

The Project Integration Architecture (PIA) is a distributed, object-oriented, wrapping architecture for capturing, encapsulating, presenting, and integrating all elements of day-to-day technical activity including, but not limited to experiment, design, analysis, simulation, and optimization.

The benefits of PIA are: fast and direct access to data of many formats, accurate capture of information, and convenient data archiving in a single environment. For more information, visit: www.grc.nasa.gov/WWW/price000

Portable Virtual Reality Environment

The portable virtual reality environment at Glenn Research Center's Graphics Visualization Laboratory allows researchers and engineers to explore their scientific data in a 3-D environment. Researchers move around in the environment using a wand and wear special "flicker" glasses to see the images in 3-D. This interaction allows the researcher to closely examine any part of their data. Virtual Reality offers interactive computer graphics that provide a viewer-centered perspective and a large field of view. For more information visit: http://gvis.grc.nasa.gov/
or http:// gruve.grc.nasa.gov/



A NASA researcher explores data from a turbomachinery simulation using the portable virtual reality environment. (NASA/GRC)

Hybrid Satellite Communications

The Transportable Earth Station (TES) is designed to support high data rate networking experiments into highly remote areas where terrestrial connectivity is poor or nonexistent. The earth station is a completely self-contained Ku-band system, able to simultaneously send and receive

Glenn Research Center:

Aviation Safety Using NPSS on the IPG

The goal of the NASA Aviation Safety Program (AvSP) is to "develop and demonstrate technologies that contribute to a reduction in aviation accident and fatality rates by a factor of five by year 2007 and a factor of 10 by year 2022."

Large volumes of flight data are collected continuously by airport flight-tracking telemetry facilities. This dataset consists of the radar tracks of all incoming and departing aircraft and could be processed to evaluate and track the engine performance of monitored aircraft. Data processing in this scenario is problematic in that it requires three basic elements: an engine simulation, high-end computing resources, and a job scheduler.

NASA Glenn Research Center has worked to provide a solution to this problem by developing a job scheduler that processes large numbers of engine simulations using the Numerical Propulsion System Simulations (NPSS). Simulations are executed on the high-end computing resources made available by the NASA Information Power Grid (IPG). For more information, visit: http://accl.grc.nasa.gov/rgriffin/AVSP/Presentation/AVSPDEMO.htm

Collecting flight data with telemetry stations for processing with Numerical Propulsion System Simulations. (NASA/GRC)

up to 50-Mbps data streams. The station is mounted on a 20-foot-long trailer and is towed by an Econoline van. No special permits or licenses are required to drive the van and trailer across public highways.

This endeavor represents a first step toward providing support for mobile and nomadic science within NASA. The

Satellite Terminal Internet Next Generation (STING) transportable earth station. (NASA)

TES can be driven to a site, parked, the antenna deployed, and the system used for satellite access to provide temporary networking facilities at that site. Potential applications of the TES include support for mobile networking technology development, workshops and conferences, scientific field studies, and international collaborations. For more information, visit: www.nren.nasa.gov

Goddard Space Flight Center

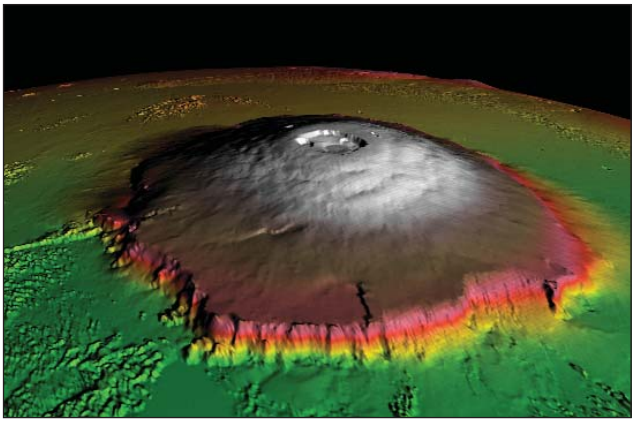
Greenbelt, Maryland

Goddard Space Flight Center (GSFC) seeks to expand knowledge of the Earth and its environment, the solar system, and the universe through observations from space. High-performance computing interprets observational data both by processing it into understandable forms and by simulating observed and unobserved phenomena.

HDTV Visualizations of Earth and Space Science

As scientists rely more on simulations and observations to understand nature, they are confronted by massive amounts of data to sift through and analyze. With data volumes at billions, even trillions of bytes visualization enables scientists to see the physical processes at work.

GSFC has created high-definition data visualizations of Earth and space phenomena. Presented in the HDTV (High Definition TV) format, visualizations shown at SC2001 include: Climate models probing the coupled ocean-land-atmosphere response to seasonal variability such as El Niño/La Niña; multi-year views of global ozone and plant



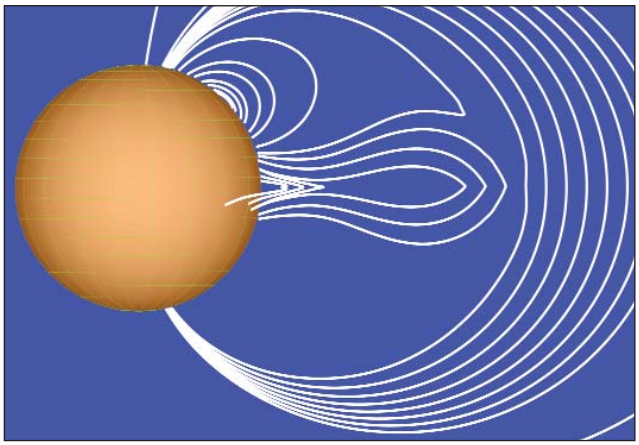
Olympus Mons on Mars. (MOLA)

life; a Mars terrain fly-over; zoom-ins to several U.S. cities that seamlessly combine four data sets. For more information, visit: http://svs.gsfc.nasa.gov

Journeys through Earth and Space

Why are the Rocky Mountains so far inland? How do we preserve the changing Amazon rain forest? When will the sun fling parts of itself towards Earth? NASA is tackling questions like these inside supercomputers. Here, billions of calculations per second recreate the universe mathematically. Supercomputers can process observations into a motion picture. Or, they can solve equations that describe realities seen and unseen.

To understand and predict nature through computation, NASA started the Earth and Space Sciences (ESS) Project,



Sun and magnetic field lines. (Goddard Space Flight Center and Naval Research Laboratory)

which is now leading the Earth Science Technology Office's Computational Technologies effort. This video magazine follows three ESS research teams on their journeys to discovery. For more information, visit: http://ess.gsfc.nasa.gov

qDoc: A Documentation and Presentation Tool

qDoc provides a means for simply documenting Fortran source code and making that documentation available via a

web browser. Documentation elements include logical source code blocks and definitions of variables, parameters, and routines.

Users insert code documentation directly into the source by means of comment characters appended with minimal character sequences describing qDoc actions. Documentation may be plain text or LaTeX commands. The code may also be sectioned into chunks for display in an expandable/collapsible HTML document format. All utilities are accessible via a user-friendly GUI enabling full or partial processing of individual or multiple files.

GLOBE Program: Multi-Agency International Educational Outreach

The GLOBE (Global Learning and Observations to Benefit the Environment) Program involves over 11,000 schools in 97 countries in observing and reporting data on environmental phenomena. The NASA GSFC GLOBE team visualizes the millions of GLOBE observations that have been reported since 1995 and makes these visualizations available on the GLOBE website.

The GLOBE visualizations can show more than 60 student datasets on the web on the same day that they are taken! Seventeen zoom levels range from whole Earth maps down to 25 x 25 km, and up to six schools or datasets can be shown on a single time graph. For more information, visit: www.globe.gov

Beowulf Technology and Applications

Beowulf-class computers are becoming the dominant architecture in parallel computing. In this demo, a number of technologies are presented that take advantage of or extend the traditional Beowulf paradigm. The Beowulf system software display showcases PVFS: The Parallel Virtual File System, a high-performance filesystem for Beowulfs, and BNT: Beowulf Network Transport, a replacement for TCP optimized for a Beowulf's internal network. The problem solving environment display showcases new areas for creating applications. The mini-grid section presents a system of interconnected Beowulfs capable of sharing resources. The Adaptive Computing Cluster display presents a merger of field-programmable gate array technology with the network interface in a Beowulf cluster. For more information, visit: www.parl.clemson.edu/

Jet Propulsion Laboratory

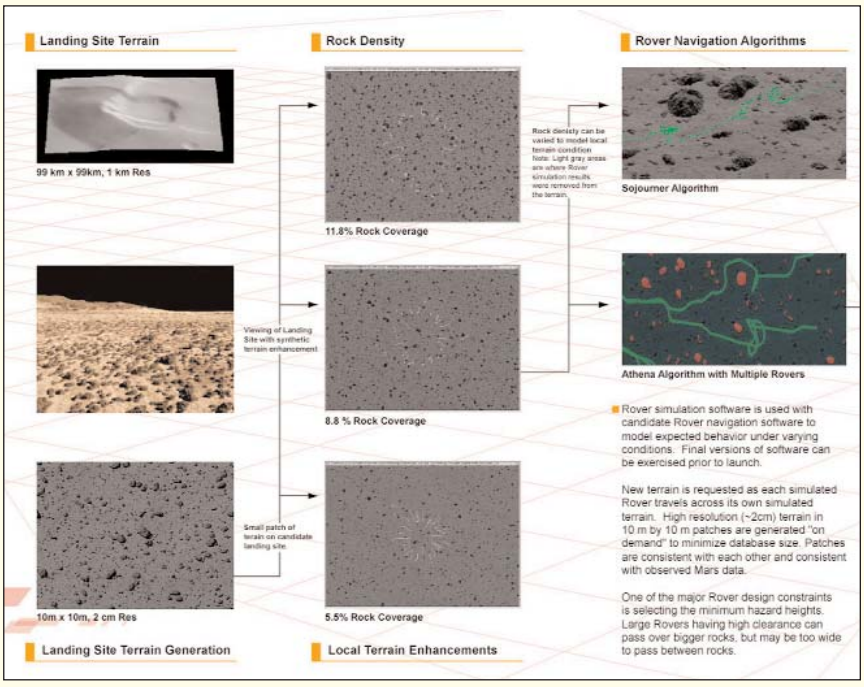
Pasadena, California

The Jet Propulsion Laboratory (JPL), managed by the California Institute of Technology, is NASA's lead center for robotic exploration of the solar system. JPL telescopes are

Jet Propulsion Lab:

Mars Site Terrain Generation Using Supercomputing

The Mars Site Terrain Generator can be used for producing high resolution (less than 1 km) site terrain based on spacecraft instrument data from prior missions. The data from diverse sources are reconciled and rendered into site models in near real time. In turn, Mars site terrain models can be synthetically enhanced with much higher resolutions (to approximately 1 cm) features to support high fidelity simulation of landing and landed (Rover) operation. Monte Carlo simulations compute the likely rover performance averaged over a large number of trials and in the presence of a large number of uncertain variables. Results from these simulations can provide valuable input for design and risk assessments.



Synthetic Mars terrain generation uses data collected by previous missions and sensors to generate terrain models, which can be enhanced to simulate landing and surface (Rover) missions. (NASA/JPL)

observing distant galaxies in the universe to study how the solar system was formed. JPL also manages the worldwide Deep Space Network, which communicates with spacecraft and conducts scientific investigations. To support NASA's continued exploration, JPL is making advances in technology with new instruments and computer programs to help spaceships travel further and telescopes see farther than ever before.

Supercomputing for the National Virtual Observatory

The National Virtual Observatory (NVO) is being built by the astronomy community, with emphasis on many interoperable components, existing in a distributed high-performance, scalable environment. The clients themselves can be anywhere and do not need specialized or high-performance capabilities.

The dramatic growth in aperture and focal plane capabilities of institutionally managed observatories has resulted in an avalanche of data, both image and catalog. NVO is conceptualized to deal with these data by developing a layered, interoperable software architecture wedded to the Internet II with its national network of computational resources. For more information, visit: http://yoursky.jpl.nasa.gov

Langley Research Center

Hampton, Virginia

In alliance with industry, other agencies, academia, and the atmospheric research community, Langley Research Center (LaRC) undertakes innovative, high-payoff aerospace and scientific activities beyond the risk limit or capability of commercial enterprises and delivers validated technology, scientific knowledge, and understanding of the Earth's atmosphere.

ISS Environment Simulator: An Immersive Application

The International Space Station Environment Simulator (ISSES) is a virtual reality application that uses high-performance computing, graphics, and audio rendering to simulate the radiation and acoustic environments of the International Space Station (ISS). The user can maneuver to different locations inside or outside of the ISS and interactively compute and display the radiation dose at a point.

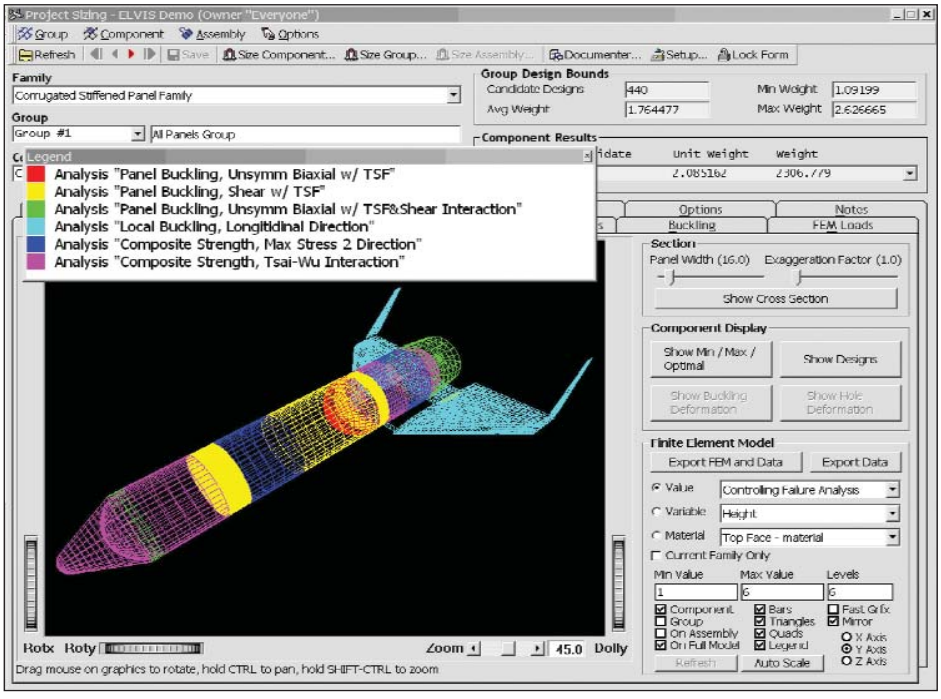
Langley Research Center:

Environment for Launch Vehicle Integrated Synthesis

At Langley Research Center, the Environment for Launch Vehicle Integrated Synthesis (ELVIS) is being developed to apply high-performance computing technologies to multidisciplinary design optimization (MDO) of Reusable Launch Vehicles (RLV).

Various discipline codes are being integrated using commercially developed framework software that allows the use of networked heterogeneous computing resources. The framework also allows easy addition or deletion of analysis codes and facilitates changes in the control flow of the MDO process through a graphical user interface.

Currently, three prototype applications are being developed: Simulation of vehicle ascent system analysis using four disciplines with parallelized trajectory optimization; computation of vehicle weights using finite element models of major vehicle structures coupled to parallel implementation of HyperSizer for structural sizing; and generation of aerothermal database and thermal protection system sizing for a complete vehicle using high-fidelity codes and coarse- and fine-grained parallelism.



Conceptual launch vehicle configuration displayed on ELVIS. (NASA)

Omnidirectional and localized sounds are rendered over headphones by a separate server that receives real-time updates on the user's position and orientation. Changes can be made to equipment rack locations, which produce changes in both the radiation shielding and system noise.

This application allows for interactive investigation and trade studies between radiation shielding and noise for crew safety and comfort. For more information, visit: http://acmb.larc.nasa.gov/

Examination of a Radiation Dose Point using the International Space Station Environment Simulator. (NASA)

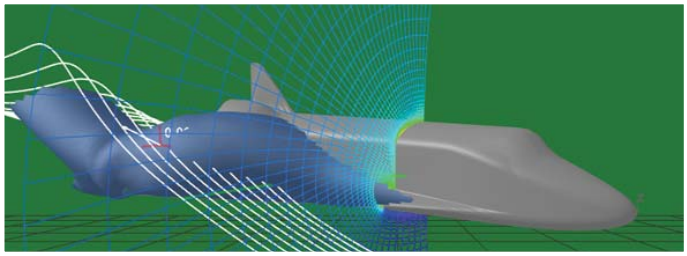
Huntsville, Alabama

Marshall Space Flight Center

Marshall Space Flight Center (MSFC) leads the Space Launch Initiative (SLI), the key to opening the space frontier for continued scientific exploration and economic expansion. SLI will make space flight safe and affordable for both the government and private industry. SLI is the centerpiece of NASA's long-range Integrated Space Transportation Plan, which also includes near-term Space Shuttle safety upgrades and long-term research and development for third generation reusable launch vehicle technologies and in-space transportation systems.

Data Visualization with Haptic Feedback

The haptic interface, one of many emerging multisensory technologies, allows the user to touch and feel computer generated models and data. The use of multisensory techniques increases the bandwidth between computers and the brain. With the haptic workstation, the user can physically interpret the nuances of a computational fluid dynamics (CFD) simulation, that is, to touch, feel, and trace the shape of phenomena such as microvortices, or secondary shock waves. For more information, visit: http://anvil.msfc. nasa.gov



Researcher wearing LCD shutter-glasses, holding haptic stylus interacts with CFD data image of a reusable launch vehicle (behind and inset). (MSFC/NASA)

NASA Participation: Presentations and Papers

Technical Papers

Tuesday, November 13
Session: Material Science Applications
1:30 p.m. to 3 p.m.

Scalable Atomistic Simulation Algorithms for Materials Research

Authors: *Aiichiro Nakano, Rajiv K. Kalia, Priya Vashishta (Louisiana State University); Timothy J. Campbell (Logicon Inc. and Naval Oceanographic Office Major Shared Resource Center); Shuji Ogata (Yamaguchi University, Japan); Fuyuki Shimojo (Hiroshima University, Japan); and Subhash Saini (NASA Ames Research Center).*

A suite of scalable atomistic simulation programs has been developed for materials research based on space-time multiresolution algorithms. Design and analysis of parallel algorithms are presented for molecular dynamics (MD) simulations and quantum-mechanical (QM) calculations based on the density functional theory. Performance tests have been carried out on 1,088-processor Cray T3E and 1,280-processor IBM SP3 computers.

The linear-scaling algorithms have enabled 6.44-billion-atom MD and 111,000-atom QM calculations on 1,024 SP3 processors with parallel efficiency well over 90 percent. The production-quality programs also feature wavelet-based computational-space decomposition for adaptive load balancing, space-filling, curve-based adaptive data compression with user-defined error bound for scalable input/output, and octree-based fast visibility culling for immersive and interactive visualization of massive simulation data.

Presentations

SGI 1,024 CPU Origin System

Presented by John Ziebarth, deputy division chief, NASA Advanced Supercomputing Division
In cooperative development with SGI, the first 1,024 processor shared memory computer was booted on July 26, 2001, at NASA Ames. By providing coherent shared memory across 1,024 processors, this system clearly pushes shared memory technology beyond previous limits. Over the past weeks, an enhanced topology for both the 512 and 1024 systems were developed with first boot in October.

MLP Scaling on NASA's Origin 1,024 CPU System

Presented by James R. Taft, Advanced Computing Technologies, NAS Division
NASA Ames has developed a very simple and highly scalable method for parallelizing a number of production applications used in critical NASA missions. The new technique, called shared memory multi-level parallelism, or MLP, is a user callable library of three routines. Scaling results for a full aircraft simulation, climate modeling, and a simulation of the space shuttle main engine all demonstrate superior performance over previous approaches.

These recent increases in code performance have had a major impact on NASA science. Highly resolved full aircraft simulations with the RANS code OVERFLOW are now done in a few hours instead of weeks. Climate predictions are 10 times faster than just a few months ago, allowing scientists to attempt simulations not possible just last year. Finally, simulations of turbomachinery for the SSME are executing 10 times faster, allowing much more detailed and timely exploration of the behavior of new designs.

Workshops

Monday, November 12 • 8:30 a.m. to 5 p.m.

Grid 2001: Second International Workshop on Grid Computing

Session V (4:15 to 5:30 p.m.) – Performance and Practice. Discussion will cover performance contracts, The DO Experiment Data Grid-SAM, and Production-Level Distributed Parameteric Study Capabilities for the Grid, which will be presented by the following NASA Ames researchers: Maurice Yarrow, Karen M. McCann, and Adrian DeVivo, and Edward Tejnil.

Panels

Friday, November 16 • 8:30 a.m. to 10 a.m.

HPC Software: Have We Succeeded in Spite of it, or Because of it?

Moderator: *John M. Levesque*
Panelists: *Walt Brainerd, Chris Doehlert, Michael Gittings, Bill Gropp, David Kuck, James R. Taft, technical director, Advanced Computing Technologies, NASA Ames.*
The moderator believes that we have succeeded in spite of HPC software. The state of HPC software is poor at best and the future of HPC software is dismal. The current thrust towards Linux and open source software does not bode well for software. This panel's discussion is targeted at a few specific problem areas such as software standards, and high performance computing software research in the academic arena.

On the cover:
Echo Lake with Mount Evans in the background. The road to the top of Mount Evans is the highest in North America climbing to 14,260 feet above sea level. The summit is 60 miles from Denver. (Richard Grant, Denver Metro Convention and Visitors Bureau)

SC2001 Booth Map

National Aeronautics and Space Administration

A • Adaptable Computing Cluster
• Beowulf System Software
• Problem Solving Environment Framework
• Computational Mini-Grids

B Data Visualization with Haptic Feedback
Space Launch Initiative Advanced Engineering Environment (AEE)

C Data Mining on the Information Power Grid (IPG)

D DeBakey Heart Assist Device

E • Mars Surveyor Landing Sites "Collaboratory"
• Unsteady Turbopump for Reusable Launch Vehicle

F IP Multicast for Seamless Support of Remote Science

G • Transportable Earth Station (TES)
• Project Integration Architecture (PIA)

H • Glenn Reconfigurable User-interface and Virtual reality Exploration (GRUVE)
• ISS Environment Simulator: An Immersive Application

I • Debugging on the Information Power Grid (IPG)
• Exploratory Computing Environments Component Framework
• Control and Observation in Distributed Environments

J growler - A Component-Based Framework for Distributed/Collaborative Scientific Visualization and Computational Steering

K • OVERSET Computational Fluid Dynamics Tools
• Parallel and Distributed CFD for Unsteady Flows with Moving Overset Grids

L • ILAB: Parameter Study Creation and Submission on the Information Power Grid (IPG)
• NAS Grid Benchmarks

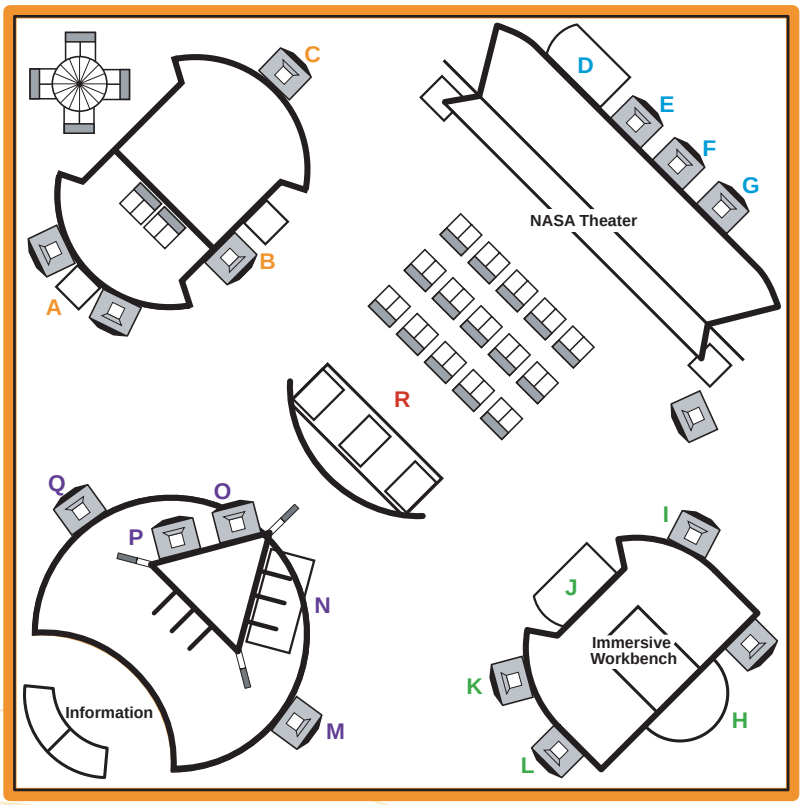
M qDoc: A Documentation and Presentation Tool

N Numerical Propulsion System Simulation (NPSS) Kiosk

O Aviation Safety Using Numerical Propulsion System Simulation (NPSS) on the Information Power Grid (IPG)

P Environment for Launch Vehicle Integrated Synthesis (ELVIS)

Q GLOBE Program: Multi-Agency International Educational Outreach



R NASA Theater – presented by: Panoram Technologies Inc.

Presentations:
• Mars Site Terrain Generation Using Supercomputing
• Mars Terrain Modeling and Rover Mission Simulation Using Supercomputing
• Supercomputing for the National Virtual Observatory
• Quantum Dot Modeling Using NEMO-3D
• IPG - A Large Scale Distributed Computing and Data Management System
• MLP Scaling on NASA's Origin 1024 CPU System
• SGI 1024 CPU Origin System
• NAS Grid Benchmarks
• growler - A Component-Based Framework for Distributed/Collaborative Scientific Visualization and Computational Steering
• HDTV Visualizations of Earth and Space Science
• Data Visualization with Haptic Feedback; Space Launch Initiative Advanced Engineering Environment (AEE)
• Glenn Research Center Video Stream

Videos:
• Journeys through Earth and Space
• Nanotechnology Video
• Powered-Lift Vehicle Simulation
• DeBakey Heart Assist Device

Field Model: Developing A Scientific Data Model

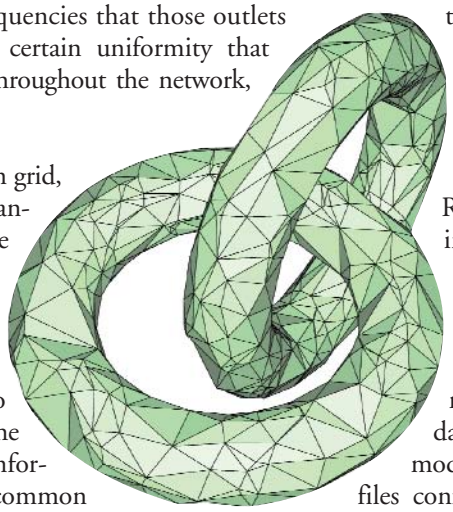
Field Model is designed to enable the sharing of data from a variety of scientific disciplines, as well as increase the reuse of analysis and visualization software components.

By Patrick J. Moran

The vision of NASA's Information Power Grid is that of an environment where high-end computing resources are as ubiquitous and easy to use as the electrical grid is today. One key aspect contributing to the success of the nation's power grid is standards: From the shape of outlets to the voltages and frequencies that those outlets provide, users can count on a certain uniformity that allows their appliances to work throughout the network, wherever they plug in.

For applications on an information grid, there are also advantages to standards. Networking infrastructure standards, such as TCP/IP (Transmission Control Protocol/ Internet Protocol), were key to the growth of the Internet. Higher-level standards, such as HTML, were also key to the explosive growth of the web. These conventions enable information exchange and provide a common model for some of the most prevalent types of meshes and fields in the information universe.

For scientific applications – especially those associated with high-performance numerical computing – some of the most widely encountered object types are meshes, and fields based on those meshes. A mesh represents a discretization of a space, a decomposition into many thousands, or in some cases millions, of smaller-sized objects known as cells. Fields are defined by associating values with the cells. In computational fluid dynamics (CFD), typical examples of fields include the momentum, density, and energy fields surrounding an aircraft. In computational chemistry, a typical area of interest would be the electron density field surrounding a molecule. Even though these disciplines may seem unrelated, the underlying commonality of meshes and fields provides opportunities for us to develop common data models. Such models in turn open the door to enhanced sharing of data and reuse of analysis software.



Researchers in the NASA Advanced Supercomputing Division are developing a software component for mesh and field data known as "Field Model" (FM), a growing library of classes written in templated C++. Built on top of the core set of classes are modules that handle various file formats and the idiosyncrasies specific to different data standards. For example, there is a PLOT3D module that makes it easy for the user to read data files conforming to the PLOT3D format, a frequently used standard in computational fluid dynamics.

FM is a follow-on to the Field Encapsulation Library, an earlier data model project (see *Learn More,* page 13). FM is

Above: *The tori are an example of one of the types of unstructured meshes that can be represented by Field Model. In a broader sense, the interlinked objects symbolize how software components, such as FM, interrelate within larger component frameworks. (Patrick Moran)*

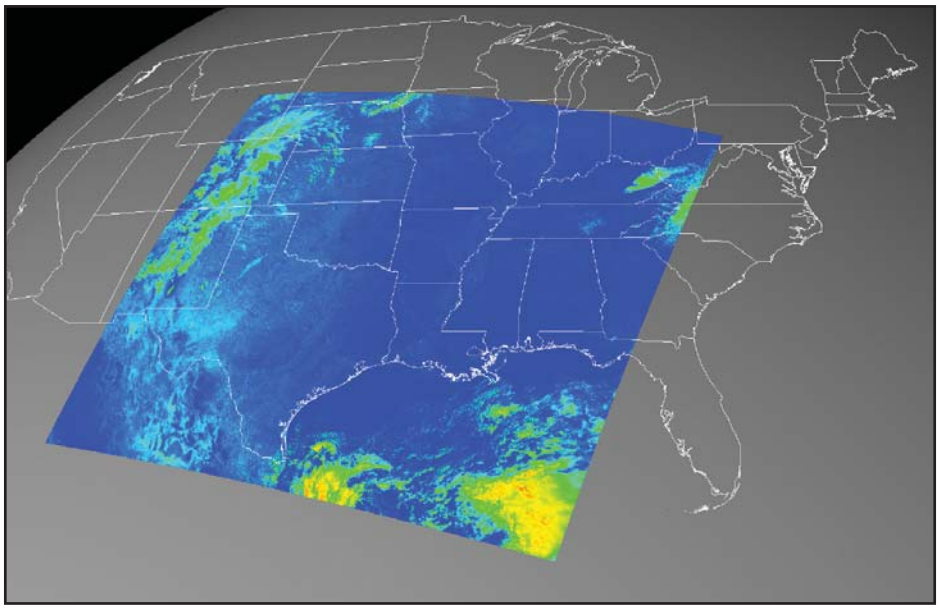


Figure 1: *The visualization of the U.S. Gulf Coast region is based upon L1B swath data acquired September 29, 2000, by the Moderate Resolution Imaging Spectrometer (MODIS) instrument aboard the Terra satellite. Terra is the flagship in NASA's Earth Observing System (EOS). The datasets are made available by the Distributed Active Archive Center (DAAC) based at Goddard Space Flight Center. (Timothy Sandstrom)*

more general and flexible than the Field Encapsulation Library, and is applicable to a broader range of data; the current effort builds on lessons learned from the previous generation of software.

Field Model as a Data Nexus

Scientists are confronted with an ever growing volume of data, from a variety of sources. A well-designed data model can help. First, a data model can provide a "common ground," in other words, a means for bringing data from a variety of sources into a common environment. This common model enables easier comparative studies. For instance, one could bring data from a variety of sensors into a single analysis application. The common model also provides advantages researchers and developers of analysis techniques. By bringing the data into a common model, more opportunities are created for applying analysis modules that may have been originally developed for one scientific discipline to another.

An excellent example of how the system works is provided by NASA's Earth Observing System (EOS) Terra satellite, which orbits the planet collecting data on a minute-by-minute basis. Data archived by the EOS is made available to scientists in an extended version of the Hierarchal Data Format (HDF) file format, which was developed jointly between the EOS program and the National Center for Supercomputing Applications (NCSA).

Figure 1 illustrates a swath, one type of data contained in HDF-EOS files. Swaths are data acquired by a remote sensor as it sweeps over a region of the Earth. FM provides modules that bridge the gap between specific file formats and the central data model. The HDF-EOS module can import EOS data into FM object instances.

Earth science data provides some relatively distinct challenges for a data model: complex projections plus a variety of numeric types, including integer types, are typical. The virtual function interface and templating features of FM address these challenges. Behind the virtual function interface, FM classes can apply routines to compute various projection transformations on the fly. Because field node types

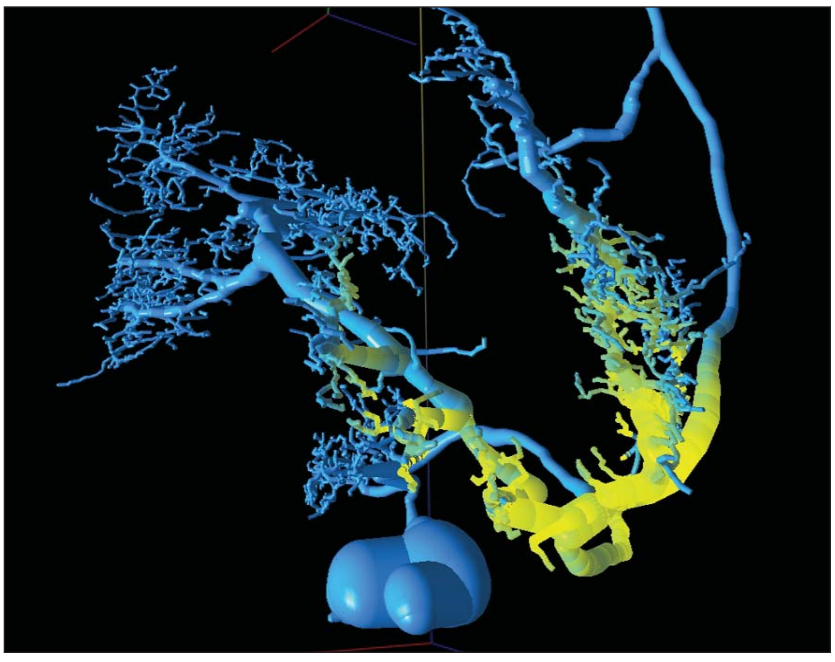


Figure 2: *This image shows a pattern of excitatory input impinging on a sensory interneuron from the abdomen of a cricket. The interneuron receives this input from a large number of wind-sensitive hair cells that create a 3D pattern of excitation (a "neural map") encoding wind direction and magnitude. The map has been idealized as a continuous excitatory field and computationally "masked" onto the interneuron using the Field Model. (Data courtesy Gwen A. Jacobs, Department of Cell Biology and Neuroscience, Montana State University; image by Chris Henze, NAS Division)*

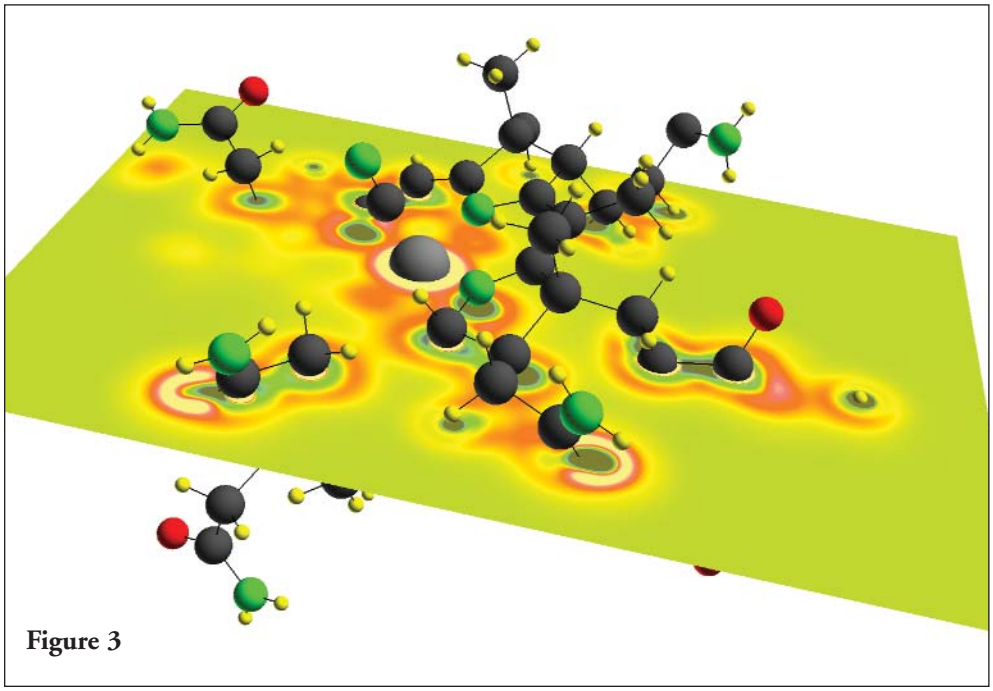


Figure 3

Figure 3, left, and Figure 4, below, illustrate two different visualizations based on the same data of a vitamin B-12 molecule. Figure 3 is a traditional ball and stick figure with a slice plane colored by the Laplacian field, while Figure 4 is a volume rendering of the same field.

The gray atom sliced by the cutting plane in Figure 3 is cobalt. The same atom is visible as a cyan sphere in the middle of Figure 4. (Figure 3: Patrick Moran; Figure 4: Chris Henze)

are templated, researchers can reuse the same FM implementations for both fixed-point and floating-point fields.

Another example of FM's versatility is shown in a molecular dataset based on vitamin B-12 (see Figures 3 and 4). In addition to molecular coordinates, the dataset includes the Laplacian (sum of the second-order partial derivatives) of the electron density field, sampled on a regular mesh in the region containing the molecule. FM includes mesh and field classes that exploit various optimization opportunities. For example, the FM regular mesh class underlying the Laplacian field provides point location and interpolation capabilities that are far more efficient than those provided for the more general curvilinear cases.

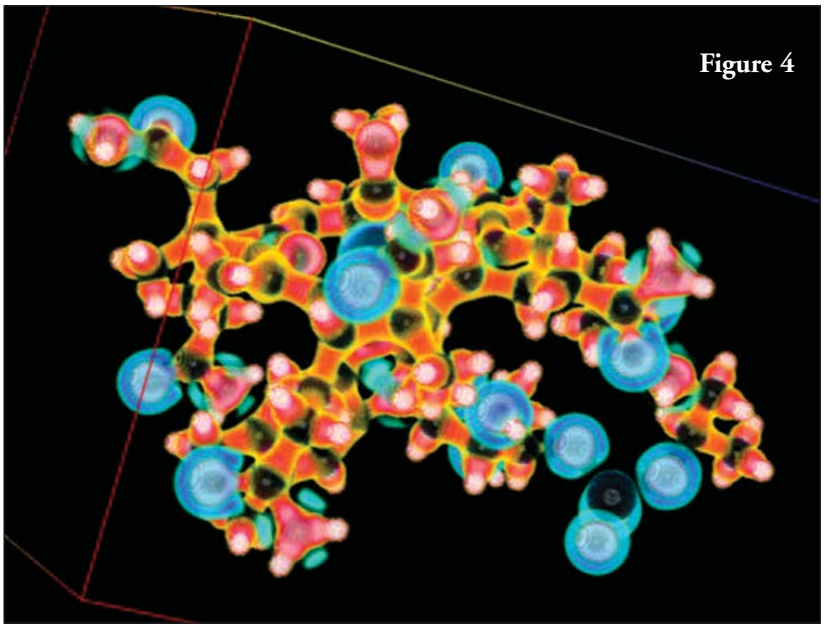


Figure 4

Object Interfaces: Generality and Specificity

The Field Model design strives for both generality and specificity. While at first it might seem as if the two goals would be mutually exclusive, both can be achieved through a combination of standard interfaces and C++ templating techniques. FM achieves generality through common interfaces for meshes and fields. The common interfaces in turn enable increased code reuse. For example, many visualization and analysis algorithms written in terms of FM work for both single and multi-block meshes. Multi-block meshes are often used when analyzing air flow in domains with complicated shapes, such as that between a wing and flaps. In some cases analysis techniques written in terms of FM also work with both structured and unstructured meshes.

The mesh interface provides iterators similar to those in the C++ standard library. Using iterators, one can loop over the cells of a mesh without regard to how the cells are represented internal to the mesh instance. Iterators further enhance reuse. For example, an algorithm designed to iterate over the vertices of a mesh can work with many different mesh types.

The majority of data access calls on FM objects occur through virtual functions where the data are requested one cell at a time. Compared to simply accessing data directly from buffers in memory, the virtual function approach comes with a minor increase in processing time. However, the virtual function interface enables the data model to handle many cases where the simpler approach would not be feasible. For example, in cases where the data are much

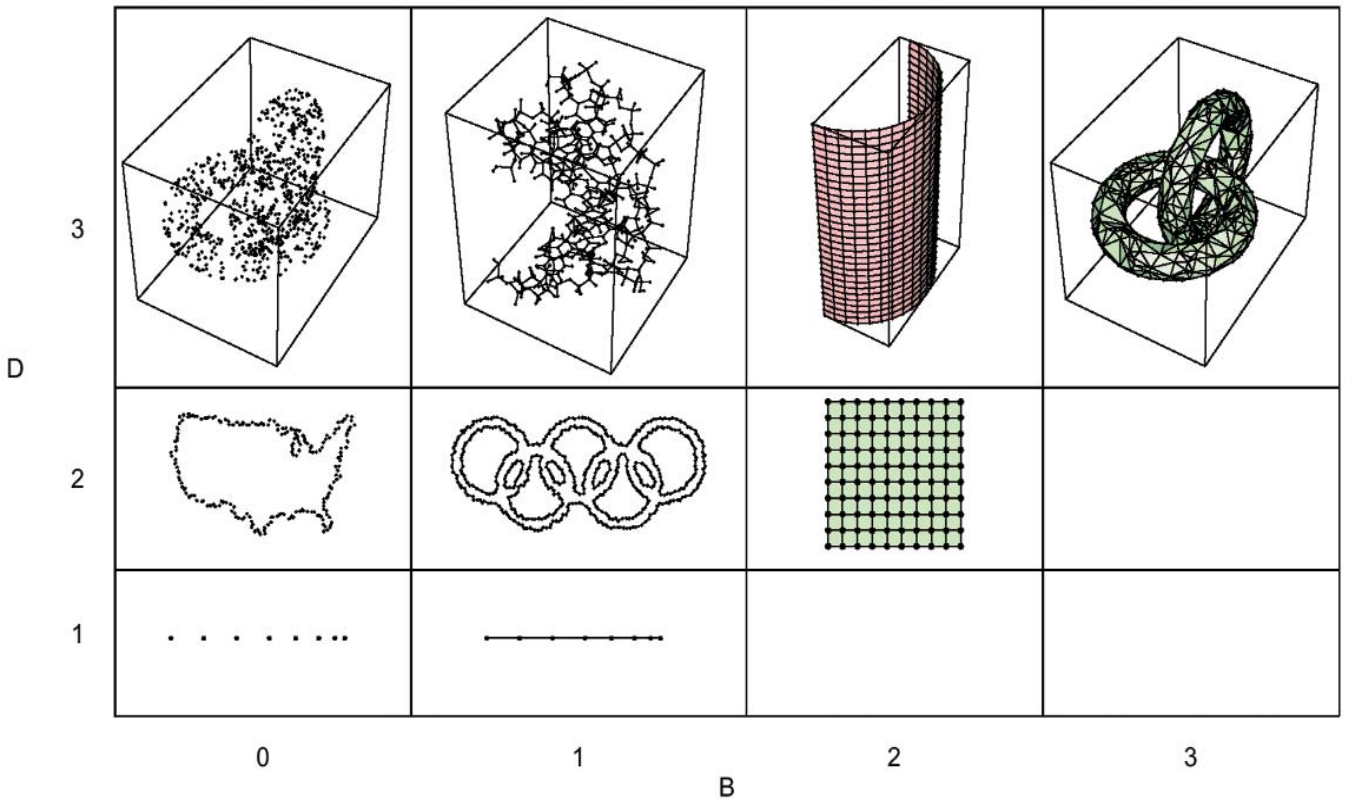


Figure 5: *Example meshes, organized by B and D values. In FM, meshes are templated by two integer parameters: B and D. The parameter B specifies the intrinsic dimensionality of the mesh shape, for example 2 for a surface, 3 for a "volume" mesh. The D parameter specifies the dimensionality of the space that the mesh is embedded in. An image object, for example, would have B and D equal to 2. An isosurface in 3-D would have B equal to 2 and D equal to 3. A hexahedral mesh in 3-D would have B and D equal to 3. Note that a wide variety of meshes can share the same templated interface, including scattered vertex meshes and molecular "stick figure" meshes. In many instances, researchers need mesh interfaces or field interfaces that are conceptually the same, but differ by specific types. For example, meshes in 2-D and 3-D have much the same interface, but differ in the number of coordinates passed as arguments. Similarly, fields all share the same basic interface, though various instances can differ by node type, for example, various scalar types (C++ captures this concept of parameterized classes through a mechanism known as templates.) (Patrick Moran)*

larger than main memory, more sophisticated techniques are required.

Demand Driven: When Laziness Is a Virtue

In the analysis of simulation results, scientists are often interested in values derived from the fundamental state variables. For example, they might be interested in velocity or vorticity values derived from the density and momentum fields output during a simulation. The approach used by older analysis tools is to compute and save the derived value over the entire field. This approach, however, can be very wasteful: in many cases the derived values are only needed on a surface, or along the path of a streamline.

A more effective approach is to compute the derived values only as needed, avoiding unused computations and saving on memory requirements. Such an approach is known as "demand-driven" or "lazy" evaluation. FM includes classes that provide lazy derived field capability. The virtual function interface of FM enables one to use lazy fields interchangeably with other types of fields, transparent to the routines accessing the data.

The lazy evaluation aspects of FM are also key to working in concert with out-of-core paging techniques. The memory requirements of eager derived fields – the opposite of lazy – would defeat the memory saving advantages of paging. With large time-series datasets in particular, it is essential that the data model have a consistent, effective strategy for memory management. In the future, NAS researchers will adapt the paging code in FEL to the FM design (see "How a New Algorithm Powers Unsteady Flow Visualization," *Gridpoints,* Summer 2001).

An Open Source Approach

FM is just one component in a larger framework development effort whose focus is interactive scientific visualization and analysis. For this effort to be a success, researchers must consider not only design issues, but also the approach to software development. For FM, the decision was made to adopt

an open source strategy. With open source software, programmers have access to the source code, enabling them to understand how the software operates. This understanding in turn allows users to contribute bug fixes and extensions, improving the quality of the software in the long run.

A data model is not a stand-alone application; rather, it is just one software component intended to serve within much larger scientific frameworks. Since the software is not self-contained, it does not lend itself to a traditional software distribution approach where ready-to-execute binary code is all that is made available. On the contrary, users need to be able to see inside the code to understand how it works to determine how it can fit within their own design. Furthermore, if other research groups are to seriously consider utilizing a component within their own software projects, there must be some assurance that licensing requirements will not require removing that component at a later time.

Working with the NASA Ames Commercial Technology Office, NAS Division researchers have established Field Model as an open source effort, based at the SourceForge software development website (see *What is Open Source?*). SourceForge is home to a vast number of open source software efforts, including projects sponsored by other government agencies, such as the Department of Energy. By embracing an open approach, the NAS Division is seeking the high-end computing community's participation and contributions. The HDF-EOS module is just one initial example of such a joint effort. Collaboration efforts are key to the success of computational science grids.

Learn More

For additional information on Field Model, Open Source, and scientific visualization, visit:

- Field Model site: http://field-model.sourceforge.net/
- Field Model: An Object-Oriented Data Model for Fields, technical report NAS-01-005. www.nas.nasa.gov/Research/Reports/techreports.html
- Open Source Initiative http://opensource.org/
- T. Sandstrom and N. Chaderjian. "The Power of Unsteady Flow Visualization." *Gridpoints*, Summer 2001 www.nas.nasa.gov/gridpoints
- The FEL 2.2 User Guide: technical report NAS-00-002. www.nas.nasa.gov/Research/Reports/techreports.html
- PITAC report: www.itrd.gov/pubs/pitac/pres-oss-11sep00.pdf
- Free Software Foundation: www.fsf.org

Patrick Moran is co-lead of the data analysis group within the Research Branch of the NAS Division. He joined NASA after receiving his doctorate in computer science from the University of Illinois at Urbana-Champaign in 1996. While at the University of Illinois he was a research assistant with the National Center for Supercomputing Applications (NCSA), where he developed high-performance biological imaging applications. His research interests include graphics, scientific visualization, and computational geometry.

What Is Open Source?

"Open source" is a designation for software intended to be distributed with source code openly available. There are a variety of licenses that have been endorsed by the Open Source Initiative as appropriate for open source distributions. The endorsed licenses are similar in that they all allow for open distribution of the initial software and redistribution of the software in modified form. The licenses also differ in crucial ways. In particular, some allow redistribution in proprietary form, while others require that all modifications remain open. Determining which requirements are essential is a topic that is still debated by industry, academia, programmers, and end users.

There are several open source efforts that are particularly relevant to high-end computing, including the GNU g++ compiler, the Python and Perl programming languages, and the GNU/Linux operating system. Among scientific visualization tools, some of the leading systems are open source, including the Visualization Toolkit (vtk) and OpenDX (formerly IBM Data Explorer). The growing importance of open source for high-end computing prompted the federal government to recently seek guidance on the topic.

A panel titled "Developing Open Source Software to Advance High End Computing" was convened by the President's Information Technology Advisory Committee (PITAC). Participants included representatives from academia, industry, and government laboratories. NASA representatives included Bill Feiereisen, chief of the NASA Advanced Supercomputing Division. The lead recommendation produced by the panel states, "The federal government should encourage the development of open source software as an alternate path for software development for high-end computing." Open source software has also been endorsed by several of the traditional vendors of high-performance computing systems, including IBM. Other information technology vendors, notably Microsoft, have argued against open source and have offered more restrictive alternatives such as "shared source" in its place.

Air Traffic Control Through Wake Vortex Management

Theories advanced by the NAS Division's Physics Simulation and Modeling Office will increase airport capacity by reducing aircraft spacing in bad weather.

When it rains in San Francisco or snows in Chicago, air traffic will be delayed. The Federal Aviation Administration (FAA) limits aircraft from flying closer than 4,300 feet to one another during the landing phase when visibility is restricted. San Francisco International Airport (SFO), for example, is unfortunately unique in that its runways are not only parallel, but are spaced only 750 feet apart. As soon as bad weather limits visibility at SFO, one of the parallel runways is closed. Runway closure reduces the airport's capacity from 95 to 99 flights per hour down to between 67 and 72 flights per hour. Depending on the length of the delay in the landing cycle, aircraft at distant airports bound for SFO are in turn prevented from taking off, as they will not have a place to land. Bad weather delays cause back-ups across the entire air traffic system.

NASA is constantly working to improve the air traffic system's capacity. The agency has been developing the Aircraft Vortex Spacing System (AVOSS) that will provide new guidelines for aircraft separation in bad weather, real-time simulations of aircraft wakes, and jetliner wake sensing and tracking. The current wake sensing and tracking components of AVOSS, however, are unable to meet the system's requirements in haze, fog, or heavy rain. Wakes are dangerous to following aircraft, and flight into a large aircraft's wake has proven fatal for many small aircraft.

To overcome the system's shortcomings in bad weather, Karim Shariff of the NAS Division's Physics Simulation and Modeling Office has filed a patent detailing a concept for sensing wakes. Shariff's research examines the interaction between large jetliners and the turbulent wakes they leave behind as they approach an airport for landing. Shariff believes that if aircraft wakes can be monitored, and detailed information about the behavior of each aircraft's wake can be provided to air traffic controllers, jetliner separations can be reduced, enabling more landings per hour in bad weather.

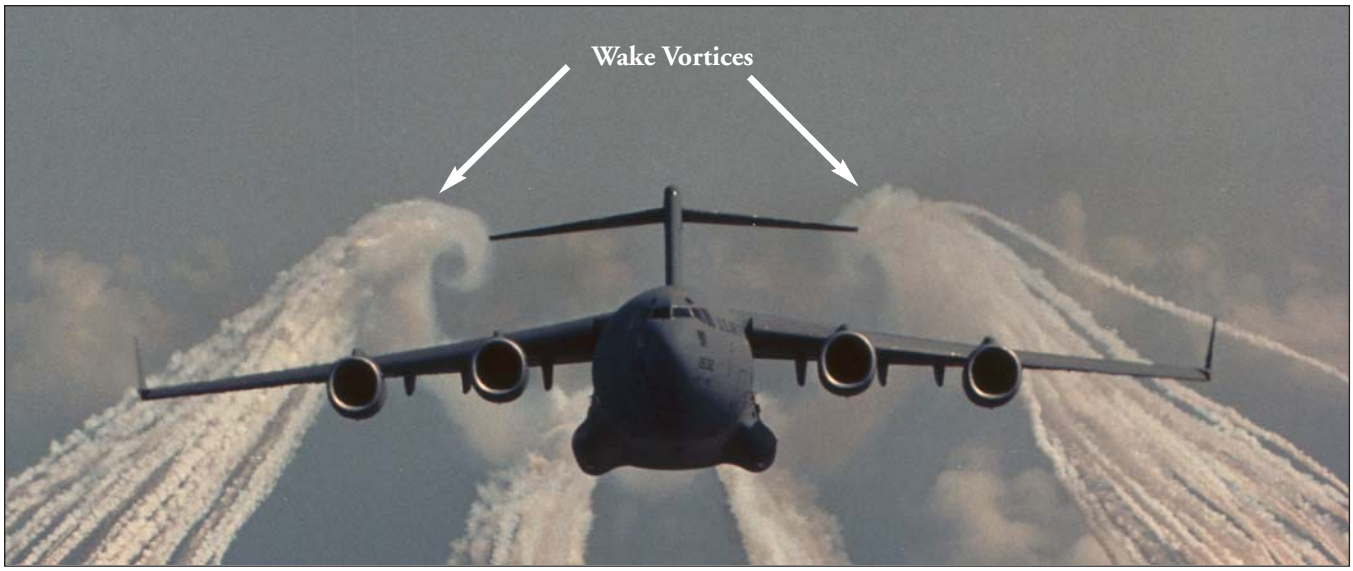
Aircraft Separation In Flight

Flight in meteorological conditions of poor visibility, such as fog, clouds, rain, or snow is known as IFR (Instrument Flight Rules). During IFR flight, pilots rely on their instruments for cues that normally come from looking out the window; for example, the aircraft's attitude in relationship to the horizon. Pilots also receive information from air traffic controllers informing them where they are in relation to other aircraft, and when to speed up or slow down during approach. Increasing or decreasing speed maintains proper spacing distances between aircraft as they near runway touch down.

Vortices are created whenever lift is generated. They are stronger when an aircraft is flying slower, and closer to the ground. When an aircraft is descending in the landing configuration – flaps deployed and landing gear down, vortices are generated as the aircraft passes through the air. The vortices combine to form a turbulent wake in the aircraft's path. Slowly, the wake descends out of the flight path and eventually dissipates. If one aircraft flies too close behind another, it will encounter the preceding jetliner's wake.

Flying through the turbulence of another aircraft's wake can cause conditions from severe buffeting – which lasts until the turbulence passes – to a loss of control. For this reason, aircraft are classified in three categories: small aircraft (less than 41,000 pounds gross takeoff weight – gtw); large aircraft, such as the Boeing 737 or DC-8 (greater than 41,000 pounds gtw); and heavy jets, such as the Boeing 747 (greater than 255,000 pounds gtw). The Boeing 757's wake turbulence is extremely strong, and although the aircraft does not meet the weight requirements to be designated as "heavy," it is classified as such for wake turbulence separations.

Having determined the dangers of following a large aircraft too closely, the FAA established a number of safety guidelines. FAA separation guidelines are applied to an aircraft flying directly behind or less than 1,000 feet below another craft as follows: "heavy jet behind a heavy jet – 4 nautical miles; large or heavy behind a Boeing 757 – 4 nautical miles; small behind a 757 – 5 nautical miles; small or large behind a heavy jet – 5 nautical miles." When an aircraft approaches the landing threshold, small aircraft are required to maintain a 6-nautical-mile separation behind a heavy jet.



Graphic representation of wing tip vortices as a U.S. Air Force Boeing C-17 airlifter flies through smoke. The aircraft's vortices pull the smoke inward as they wrap around each other. The C-17 is in the same "heavy" class as the Boeing 747 jumbo jet. (Boeing)

Many researchers and experts in the airline industry believe the FAA-mandated separations are too conservative. The FAA believes: "$5 billion could be saved annually by the airlines if one could safely reduce the current separations by 1 nautical mile." Aside from the financial gains, flights would be safer, and passengers would arrive at their destination sooner.

Today's Wake Vortex Tracking

NASA currently uses LIDAR (LIght Detection And Ranging), a laser-based device that sends an infrared beam into the wake of an aircraft for wake detection. Naturally occurring aerosol particles scatter the beam back to the device, which is able to determine the position and speed of the particles. LIDAR, considered a first-generation vortex detector, has a number of drawbacks when viewed as a potential field-installed system: infrared particles are absorbed in water vapor, rendering the system inoperative during foul weather; and as an optical system, it requires a high amount of maintenance, including cleaning and replacement of optical parts; and it is expensive to acquire and operate.

LIDAR was tested in Memphis, and has subsequently been installed at Dallas/Ft. Worth International Airport. The system has proven that it can measure aircraft wakes and determine velocity profiles. The continuous wave LIDAR has a range of only 900 feet – inadequate for a production system – and the high-power pulse LIDAR is only capable of detecting vortices out to 2.5 miles in clear weather. LIDAR's success will hopefully convince the FAA that the concept is viable, which will enable NASA to secure funding to develop a next-generation system.

Patenting A Theory

Shariff's theory suggests that radar is a feasible next-generation wake detection system. Using radar, rather than an optical system, to detect wakes gives an all-weather capability. "Radar scattering analysis revealed that peak reflectivity from a trailing vortex occurs at a frequency near 50 megahertz (MHz) (see Figure 1), and is strong enough that a vortex could be detected at a 3 kilometer range with an average power of about 400 watts," says Shariff. "A frequency of 50 MHz has several advantages: Clutter from rain and fog is not an issue and so the system would work in all types of weather; inexpensive and low-maintenance radars already operate at 50 MHz for measuring atmospheric winds, and they could be modified to track vortices; and, if the system is supplemented with sound waves to enhance reflectivity, the required sound frequency is low enough that attenuation of the sound wave (which would limit range) is not a problem."

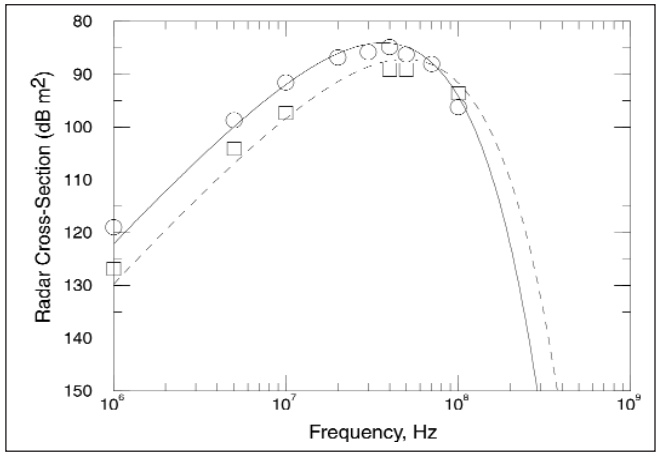


Figure 1: *Predicted radar cross-section (RCS) of aircraft vortices. The symbols show the results of a scattering analysis implemented computationally. The curves show the results of a simple but approximate analytical formula. Solid line and circle symbol: Vortex RCS for heavy class (Boeing 747) aircraft. Dotted line and square symbol: Vortex RCS for a large class (DC-8) aircraft. This figure is for a range of 1 kilometer.*

(Karim Shariff)

NASA's Langley Research Center performed a number of wake vortex studies at its Wallops Island facility. A crop duster was flown low and slow over a red smoke flare. As the wing tip passed over the smoke generator, the vortices created a turbulent flow that can cause control problems to following aircraft. (NASA)

Based on this theory, Shariff has filed a provisional patent that states wing tip vortices can be detected at 50 Mhz by making modifications to existing ST radars (Stratospheric, Tropospheric; such radars are used for atmospheric physics). "It's a unique patent in the sense that it claims that such devices exist already, and that with some modification they can be used for a different application," Shariff explains. "It's not that I have a new device, it's more of a concept. That's why there was some reluctance about patenting it given that it is another application of an existing device. But given that it is another application of an existing device, and given that it needs to be modified, hopefully they'll give the final patent and then I can say how one would go about modifying it."

In an implementation of the radar device, air traffic controllers would be able to view data from the 50 Mhz radar, detect the position of the vortices of landing aircraft, and then inform trailing aircraft whether they should speed up or maintain current spacing. The 50-Mhz radar would use approximately 30 Yagi-type directional antennas (a pair of dipoles, a parallel reflector, and a set of directors) arranged in a "farm" near the end of a runway.

Putting the Theory to the Test

Shariff plans to put his theory to the test at Vandenburg Air Force Base, California, within the next year. The U.S. Air Force has built an Airborne Laser for use in destroying Scud-type, tactical theater missiles during the boost phase. The Airborne Laser has been mounted into a 747-400 freighter that will orbit over battlefields and destroy missiles as they ascend.

The Air Force plans to test the Airborne Laser over the atmospheric radar range at Vandenburg. "They will be looking at the deflections of this airborne laser beam due to atmospheric turbulence. And then they'll compare the data with measurements on atmospheric turbulence they get from the Vandenburg radar and use that to correct the beam's path," Shariff says. "I've asked them if I can do a test in the wake as the aircraft flies past this radar. The atmospheric radar is exactly the same frequency as my predicted 50 Mhz.

Shariff has received approval to run his experiment in concert with the Air Force program. Once he obtains the test results from Vandenberg and has his patent in hand, Shariff will begin developing the system, which will require analyzing wakes of other aircraft classes in a variety of weather conditions. The size of the radar's antenna farm, and the beam's coverage of a typical landing approach path will also have to be determined. Once developed into a field deployable system, NASA will transfer the technology to industry.

"We're pursuing this research because building more airports is not really an option," Shariff says. "Environmental issues, such as noise pollution and habitat encroachment, as well as real estate costs, make building new airports prohibitive. It is making use of wasted airspace, and it's wasted because of these vortices."

— Nicholas A. Veronico

Calendar of Events

Ninth Foresight Conference on Molecular Nanotechnology

Santa Clara, California • November 9–11

The Ninth Foresight Conference on Molecular Nanotechnology will be held at the Westin Hotel in Santa Clara, California to provide a forum for leaders from all areas of science and technology involved in research at the nanoscale to present and discuss their most recent results and ideas. Visit: www.foresight.org/Conferences/MNT9/index.html

SC2001

Denver, Colorado • November 10–16

SC2001 will bring together scientists, engineers, designers, and managers from all areas of high-performance networking and computing, and showcase the latest in systems, applications, and services. The conference website is: www.sc2001.org

2001 Information Power Grid Workshop

Palo Alto, California • December 5–6

This year's workshop will be held at the Crowne Plaza Cabana Hotel, in Palo Alto, California, to focus on IPG-related grid technology. Presentations will include talks from research and development teams from each of the major IPG-related organizations including: NASA centers; Argonne National Laboratory; NCSA; San Diego Supercomputer Center; USC's Information Sciences Institute, and other participating universities. Papers in several areas are being solicited for presentation and discussion at the workshop. Advance registration is required. For the latest information, visit: www.ipg.nasa.gov or NAS's technical training site: www.nas.nasa.gov/User/Trainng/training.html. For more information, contact: Marcia Redmond, mredmond@mail.arc.nasa.gov.

Global Grid Forum (GGF) Four

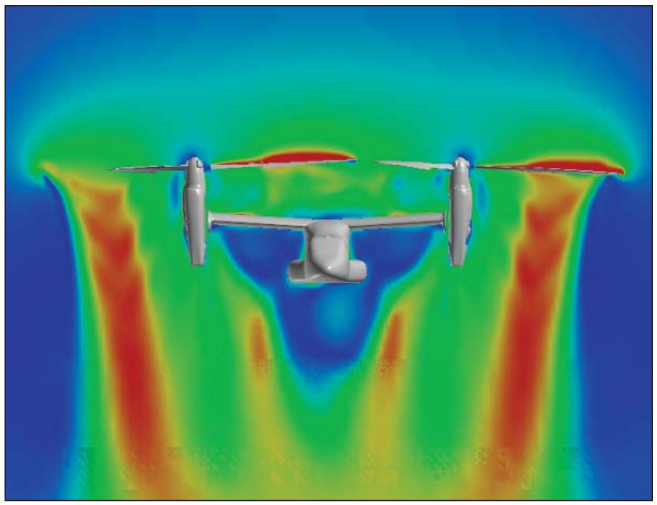
Toronto, Canada • February 17–20

The fourth Global Grid Forum provides working and educational sessions for researchers and those interested in grids and grid technologies. Agenda and details are coming soon to: www.gridforum.org

IEEE Virtual Reality 2002

Orlando, Florida • March 24–28

Research and technology exhibition showcasing virtual reality software, hardware, and systems development. The seventh annual Immersive Projection Technology Symposium will be held inconjunction with the virtual reality exhibition. Additional details are available at: www.VR2002.org



NAS Division researchers have developed a parallel and distributed computing (PDC) tool for large-scale unsteady moving body applications using overset structured grids. The V-22 simulation is a large-scale Navier-Stokes problem consisting of a moving body grid system of approximately 37 million points. A performance assessment of the PDC tool indicates that this application can be run on wide area networks such as NASA's Information Power Grid. (Jahed Djomehri)

IEEE Symposium on Mass Storage Systems

Adelphi, Maryland • April 15–18

The 19th IEEE Symposium on Mass Storage will be held in cooperation with the 10th NASA Goddard Conference on Mass Storage Systems and Technologies at the Inn and Conference Center at the University of Maryland to provide a forum for discussion of issues relevant to the management of large volumes of data. For more information visit http://storageconference.org/2002

International Parallel and Distributed Processing Symposium

Ft. Lauderdale, Florida • April 15–19

The International Parallel and Distributed Processing Symposium (IPPS/SPDP) is designed for scientists and engineers from around the world to present their research and discoveries in all aspects of parallel computation. The symposium will include technical sessions, workshops, tutorials, and commercial exhibits. For conference information, visit: www.ipdps.org

Siggraph 2002

San Antonio, Texas • July 21–26

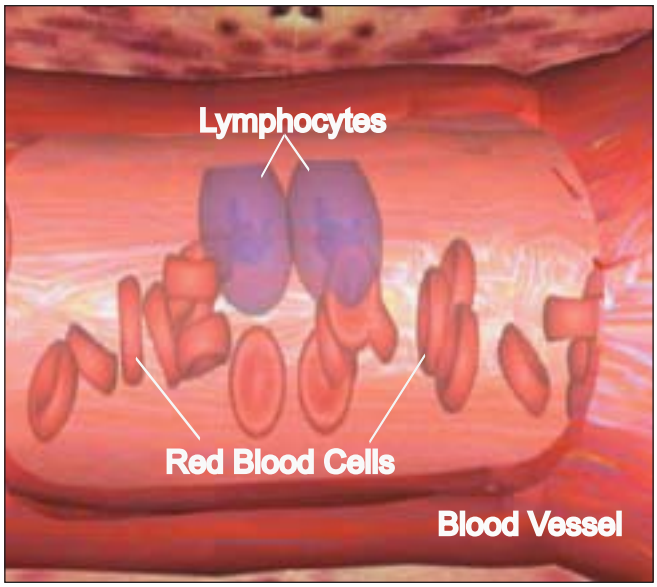
The 29th International Conference of Computer Graphics and Interactive Techniques is a forum for computer graphics scientists, artists, engineers, and educators. Technical presentations will include papers, panels, courses, applications, an educators program, web graphics program, and an applications lab. Conference information can be viewed at: www.siggraph.org/s2002

National Aeronautics and Space Administration
NASA Advanced Supercomputing Division
Ames Research Center
MS 258-6
Moffett Field, CA 94035-1000

FIRST CLASS MAIL
POSTAGE & FEES PAID
NASA
Permit No. G-27

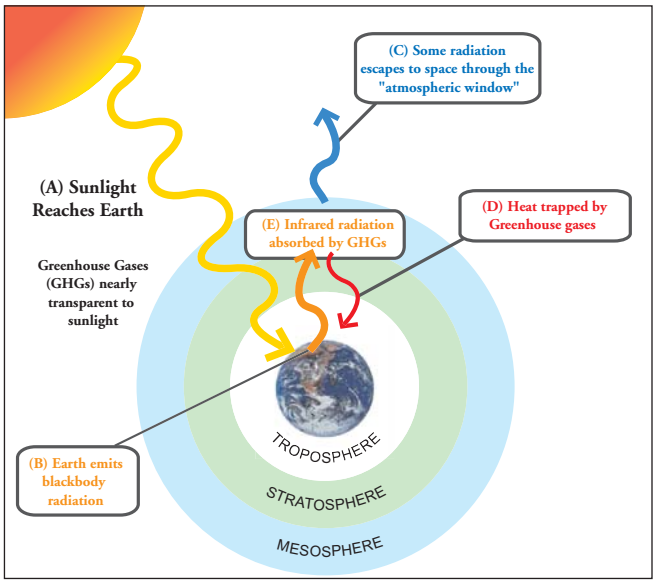
Official Business
Penalty for Private Use $300

Address Correction
if the above address or mail stop is incorrect, please e-mail a current address to gridpoints@nas.nasa.gov, or write to:
Gridpoints Editor, MS 258-6, Moffett Field, CA 94035



Solving The Cancer Equation

A visiting professor at the NAS Division believes the key to winning the war against breast cancer is using partial differential equations to model the spread of cancer in individuals. See page 4.



The Heat is on . . . Earth

Computational Chemistry is being used to calculate the level of toxicity of industrial compounds being released into the Earth's atmosphere, which are contributing to a rise in global surface temperatures. See page 6.